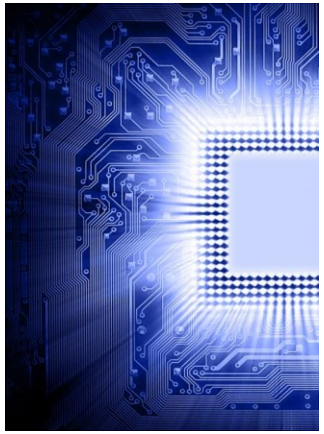
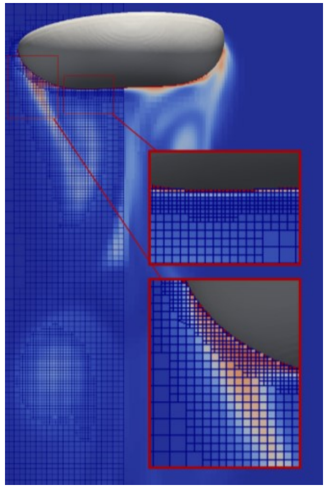




Parallelization of CFD Simulations

Dr.-Ing. Holger Marschall

High Performance Computing for Simulation Science

Learning Objectives of Today‘s Lecture

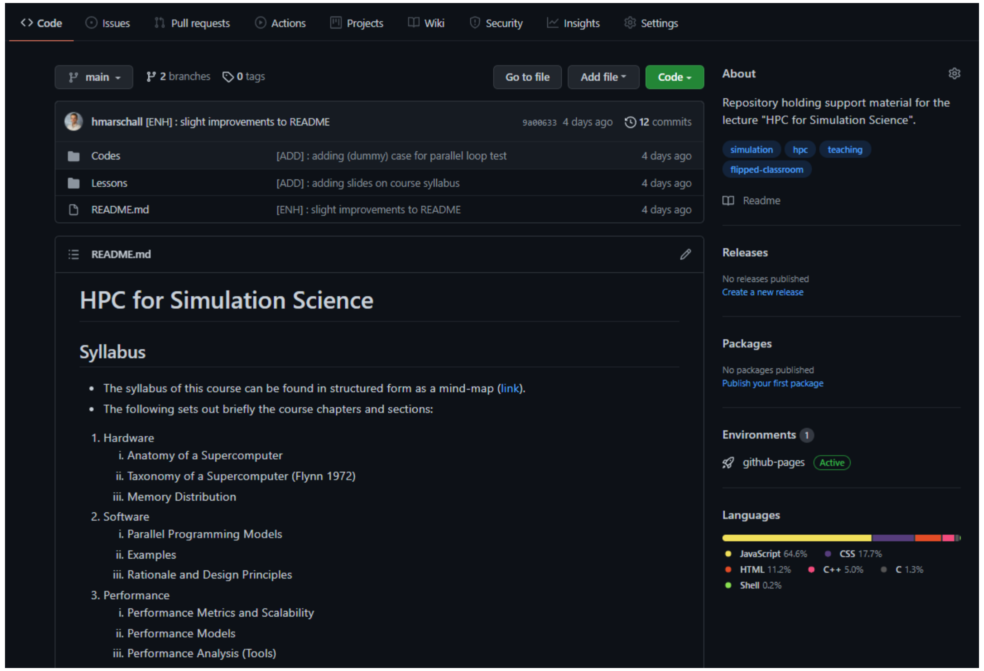
Students understand…

- the categorization and relevant combinations of **Parallel Computing Models**
- the conceptual differences between **Data and Task Parallelism**

Students are able to …

- detail on the application of suitable **HPC techniques for Parallel Computational Fluid Dynamics**

Please fill the Worksheet 2.2 during the lecture!



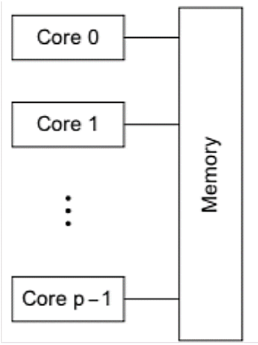
Support material online!
https://bit.ly/HPC4SimulationScience

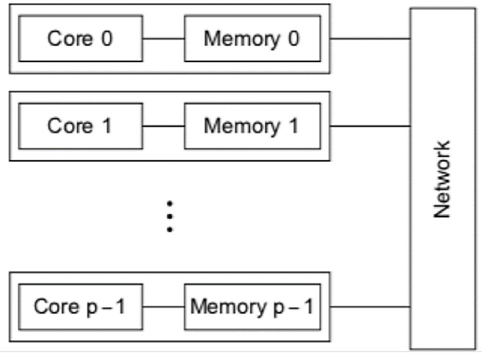
```
🗁 Assigments/
🗁 Codes/
🗁 Lessons/   ←
README
```

01 Summary

Parallel Programming Models

Shared vs. Distributed Memory





Shared:
all processors
- share same addressing
- access a pool of shared memory

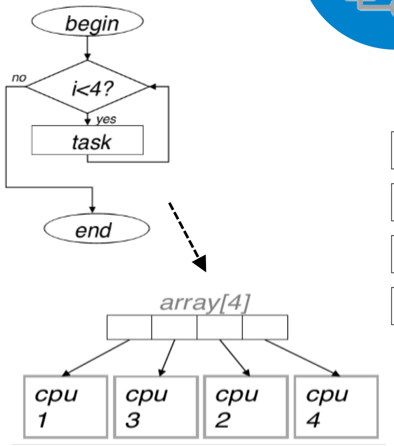
Distributed:
each processor
- with own local memory
- message passing for communication

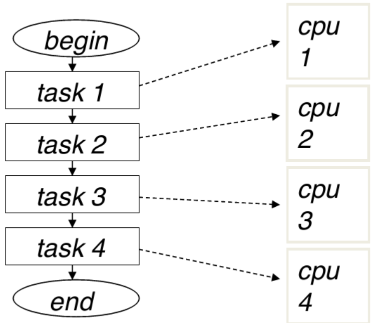
Explicit vs. Implicit

Explicit:
Explicitly expressed in the source code by the program developer

Implicit:
Implicitly (automatically) identified by the compiler

Data vs. Task





Data:
- divide into sub-groups
- assign each piece to diff. processors

Task:
- divide algorithm into functional pieces
- execute each piece on separate processor

02 Distributed Memory Model with Explicit Data Parallelism

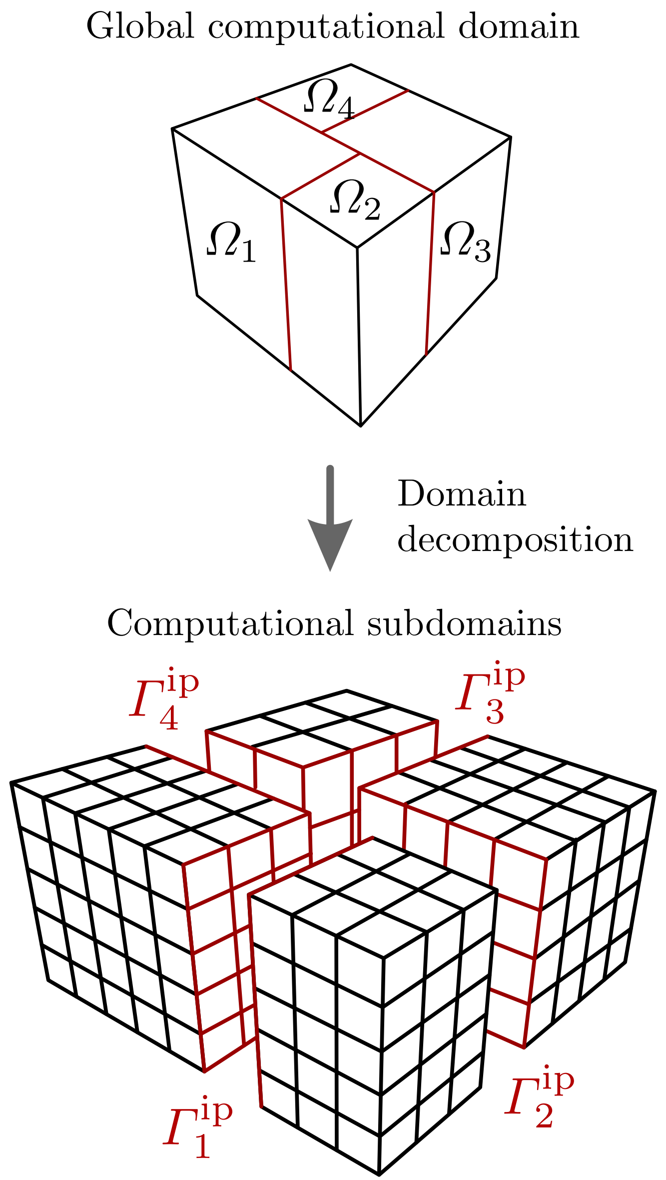
Example: Parallelization in CFD Simulations

Parallel CFD simulations require the following essential steps:

- **Domain Decomposition**
  Task: Decompose the computational domain into sub-domains, viz.

  and the mesh/field data accordingly.

- **Parallel Communication**
  Task: Devise a mechanism for data transfer across inter-process boundaries.



📖 Ferziger, J. H., Perić, M., & Street, R. L. (2020). Computational Methods for Fluid Dynamics. Springer International Publishing.

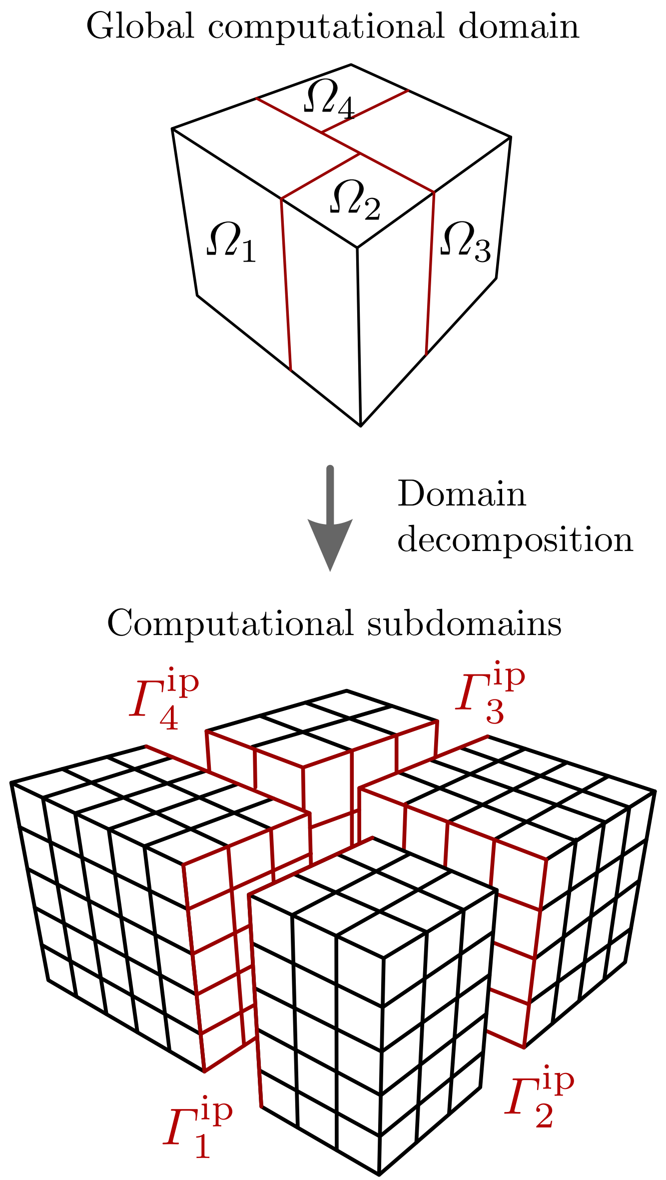
02 Distributed Memory Model with Explicit Data Parallelism

Example: Parallelization in CFD Simulations

Parallel CFD simulations require the following essential incredients:

1. Domain Decomposition Strategy

- each cell uniquely allocated to separate processor
- same set of operations performed over all mesh sub-domains
- each processor runs a copy of the solver on a separate part of the decomposed domain



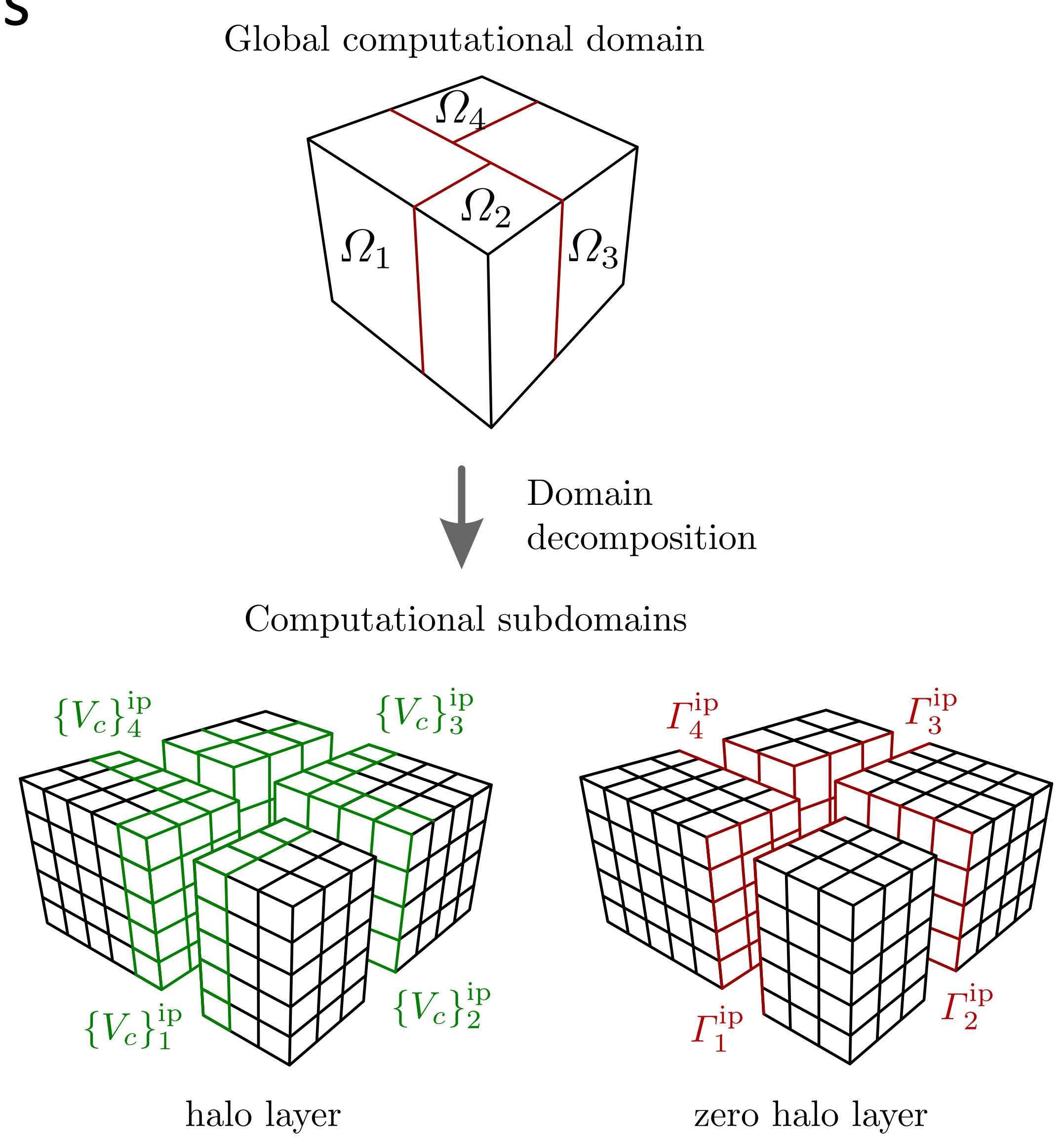
02 Distributed Memory Model with Explicit Data Parallelism

Example: Parallelization in CFD Simulations

Parallel CFD simulations require the following essential incredients:

2. Parallel Communication Device

- *Halo Layer* approach
  cell data next to processor boundary is duplicated, explicitely updated via parallel communication calls
- *Zero Halo Layer* approach
  no dublication, inter-processor communication established as boundary condition



03 Parallelization in CFD Simulation

Parallel Communication: Zero Halo Layer

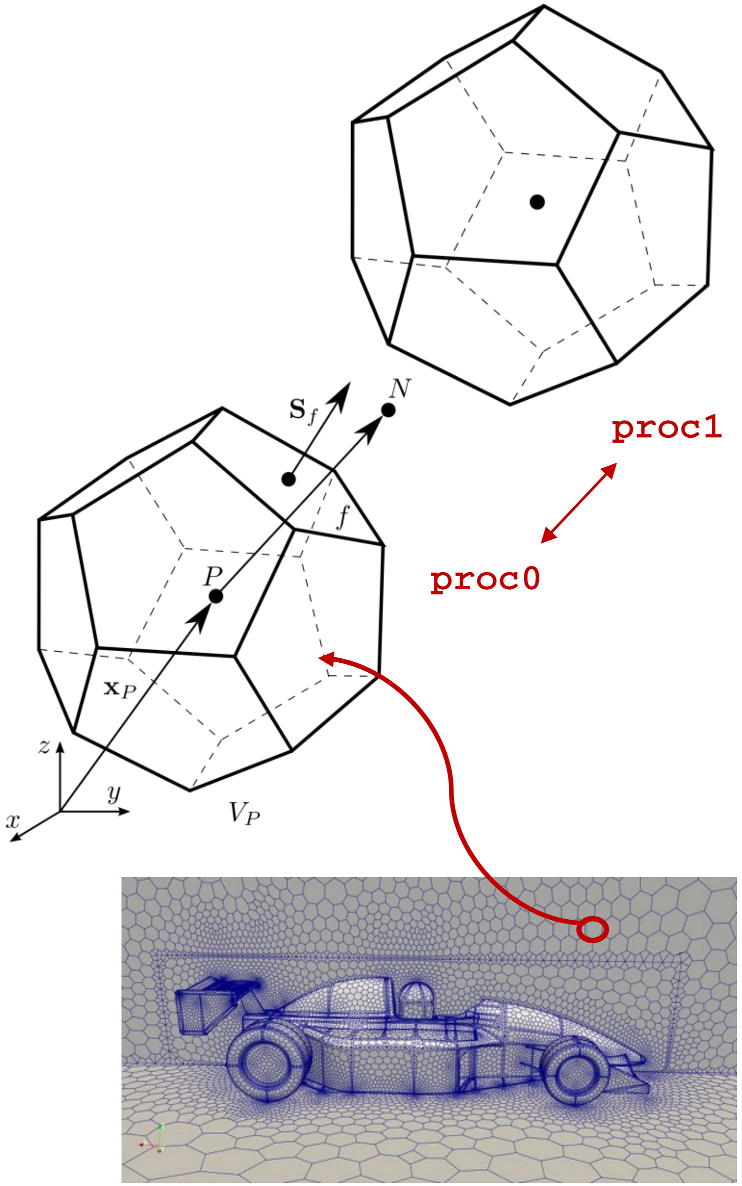
- **Finite Volume Matrix Assembly**

Consider a generic transport equation:

$$\partial_t(\rho\phi) + \nabla \cdot (\rho \mathbf{u} \phi) - \nabla \cdot (\Gamma \nabla \phi) = S_\phi(\phi).$$

⤳

⤳



– Assembling the matrix coefficient for advection and diffusion terms requires *exchange of geometrical and interpolated field data.*

Example: off-diagonal matrix coefficient for diffusion operator:

$$a_N = \Gamma_f \frac{|\mathbf{S}_f|}{|\mathbf{d}_f|}$$

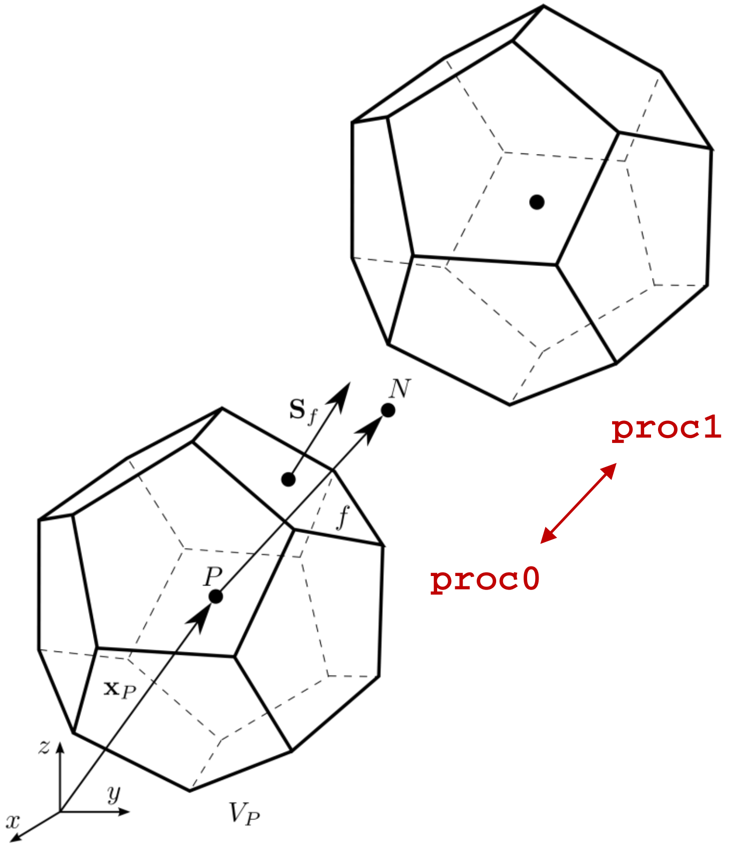
– Sources/sinks and temporal terms do not impair communication.

03 Parallelization in CFD Simulation
Parallel Communication: Zero Halo Layer

- **Communication Pattern: simple pairwise**

  1. Collect relevant cell values and geom. data from local subdomain and **send** to neighbour processes
  2. **Receive** neighbour values and geom. data from neighbour processes
  3. Interpolate values and use geom. data to **assemble** matrix coefficients

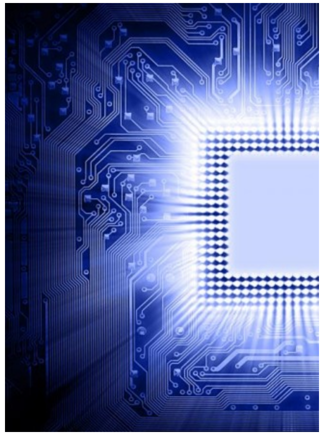
  → Message passing library: MPI (de facto standard)

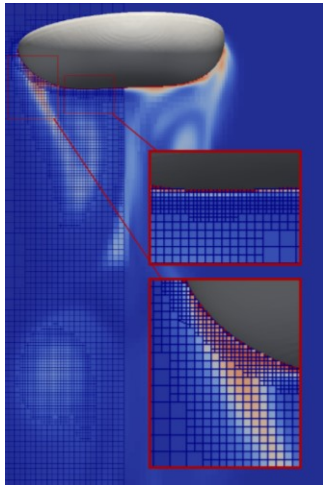


MPI Forum, MPI: A Message-Passing Interface Standard Version 4.0, Technical Report 2021.

Next Lecture & Plenum Events

- **Next Lecture:**
  Shared Memory Model with Explicit Task Parallelism
  (Force Decomposition in Parallel Molecular Dynamics)
- **Next Plenum:**
  Question & Answer, Peer Instruction
  (Exercise, see online support material)





Thank You for Your Attention!

Note your questions on the worksheet for the plenum event!