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Models, Math, Data, and Computing - Computational Science at USI

R. Krause

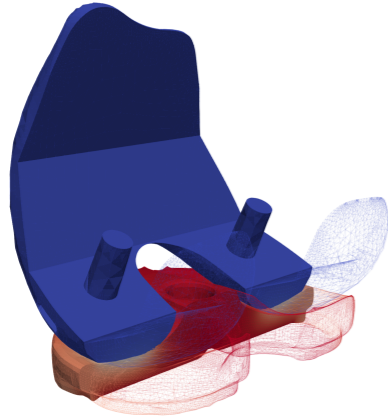
A. Auricchio, S. Bader, P. Benedusi, V. Braglia, L. Gaedke-Merzhäuser, A. Gharaviri,
A. Kopaničáková, C. Tomasi, M. Nestola, S. Pezzuto, C. von Planta, P. Zulian, L. Belluzzi,
S. Riva

**Euler Institute
USI**

Università della Svizzera italiana, Lugano

Lugano, 3.9.2022

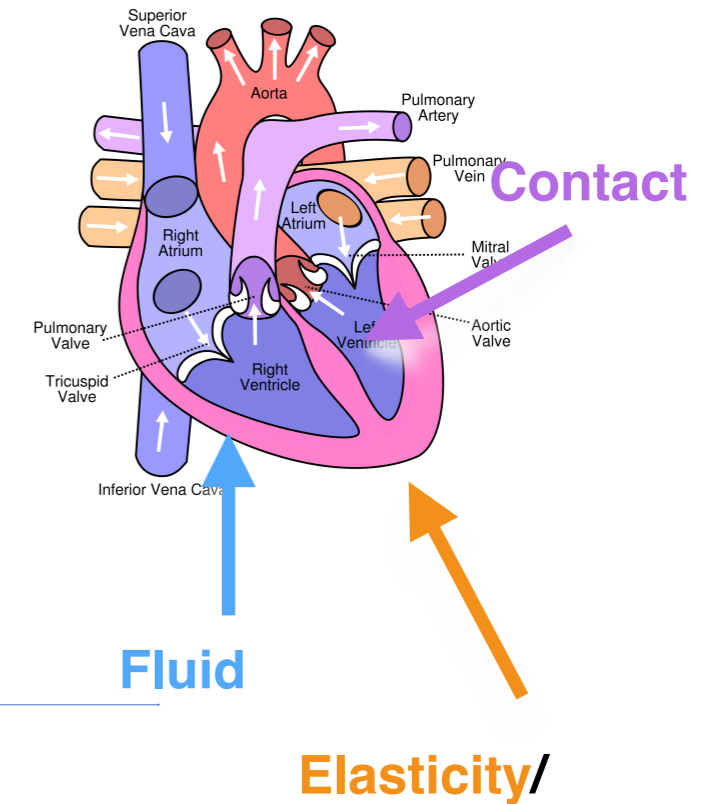
Computational Mechanics



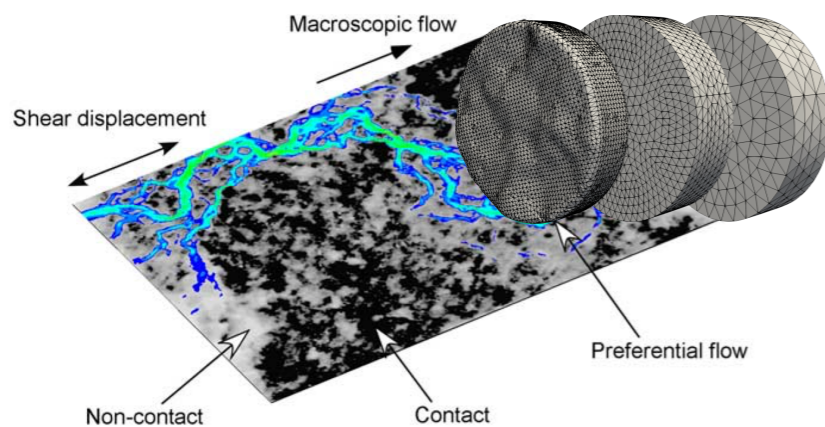
High-performance computing



Computational Medicine



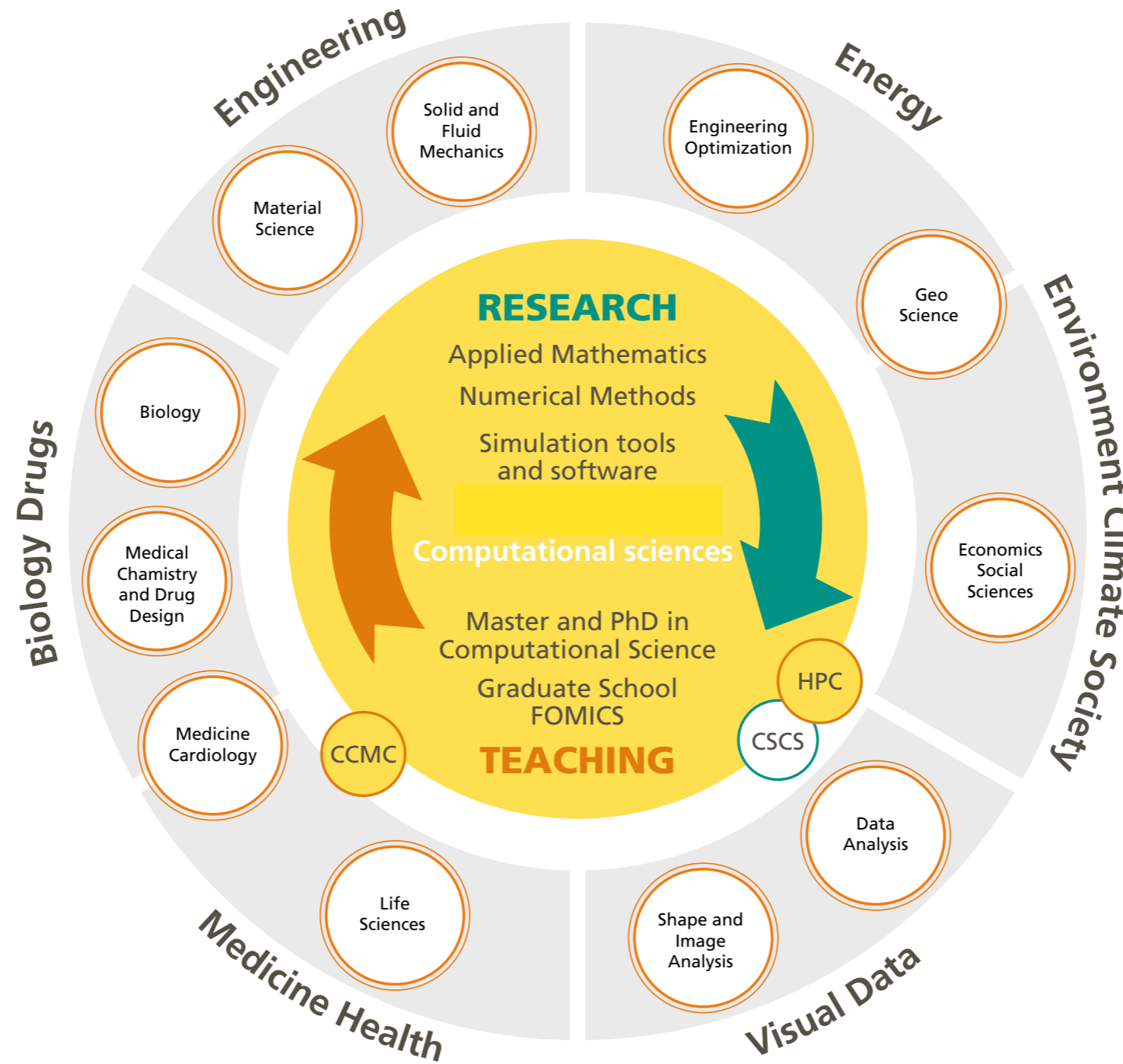
Abstraction
Provides
Flexibility



Computational Geophysics

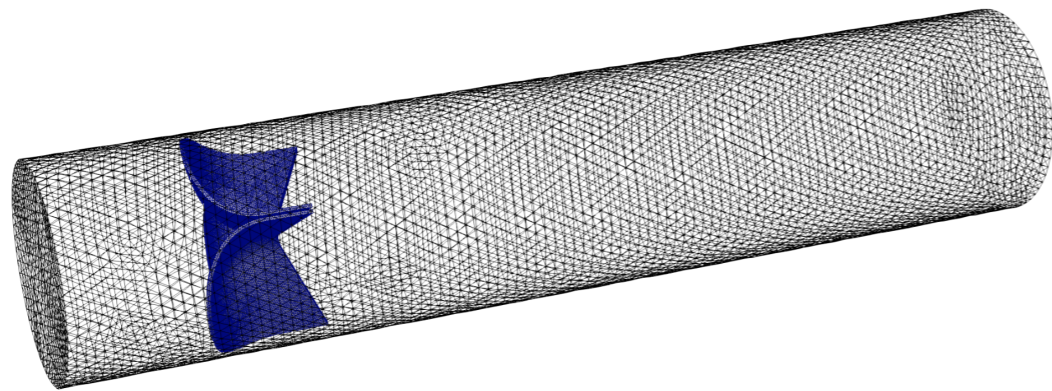
Machine Learning

Cloth simulations for animation



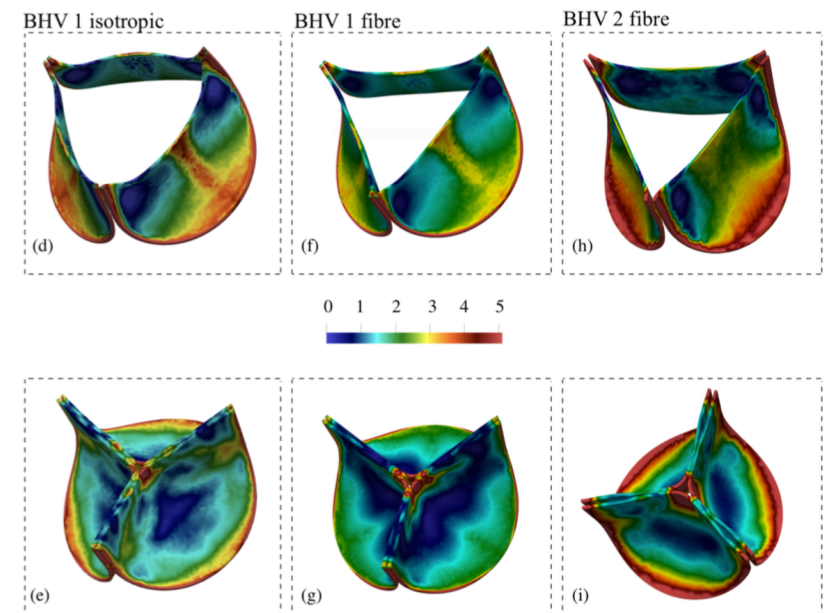
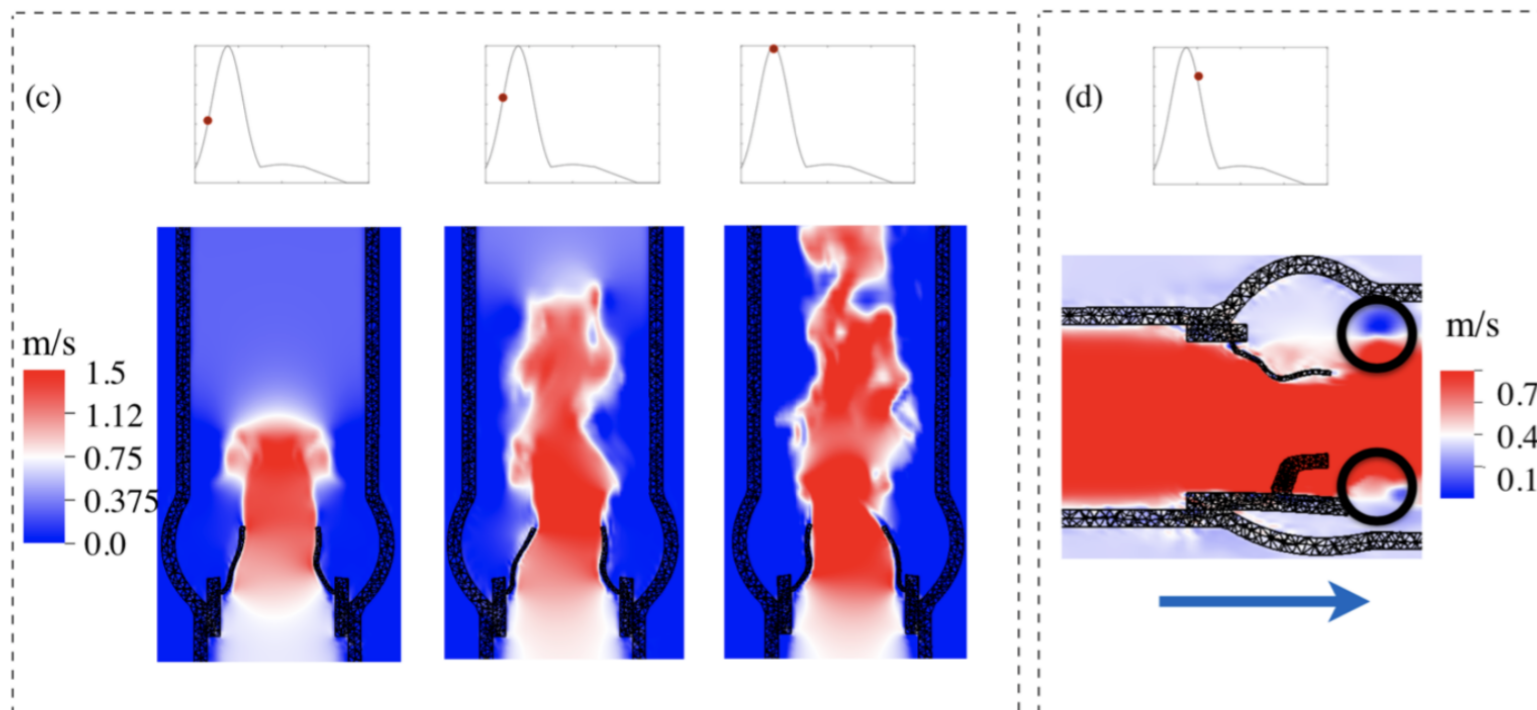
Multiphysics - Bioprosthetic Heart Valve

Immersed domain → fluid and solid are coupled in the entire intersection volume



FSI-contact simulation

- Mechanical and haemodynamic performance
- (a) Velocity. Inflow boundary condition.
- (b) Windkessel model for pressure gradient between 80 and 120 mmHg
- (c) Systole
- (d) Diastole



Lagrange multipliers

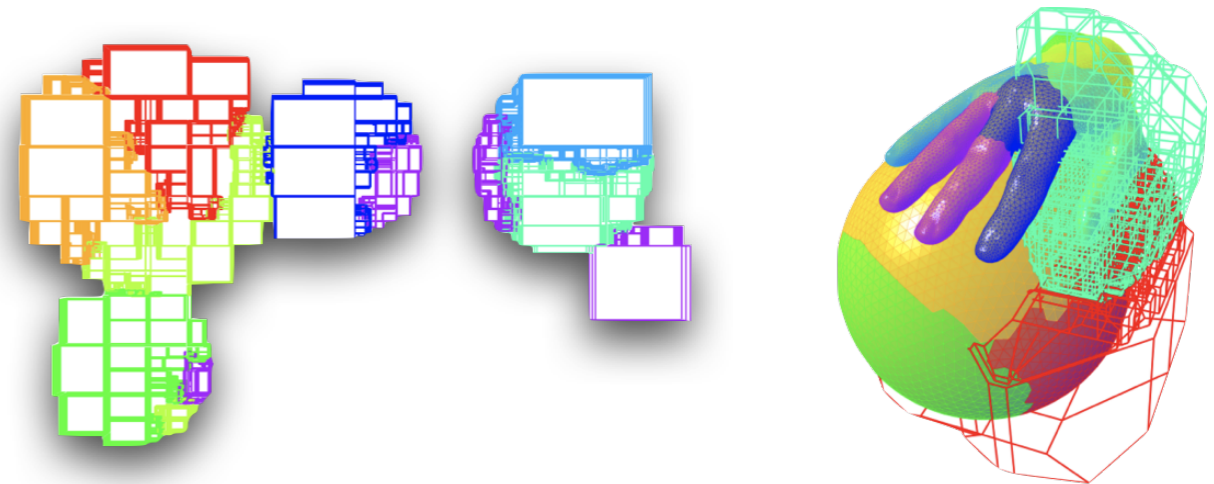
Method of Lagrange multipliers

- **FSI** terms (**Volumetric** coupling)
 - **Contact** conditions (**Surface** coupling)
 - Transfer of information between **solid** and **fluid** discretizations
- In this presentation both use **FEM** or **CVFEM**



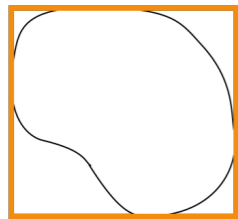
Geometric operations

- **Solid** is considered in the **deformed/physical configuration**
 - Mesh **entity relationships** have to be determined
- Geometric search using space partitioning techniques (MPI based bounding volume hierarchies)

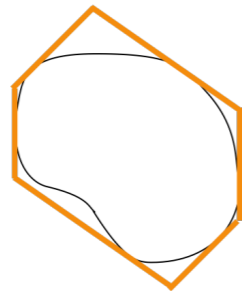


Variational transfer: parallel algorithm

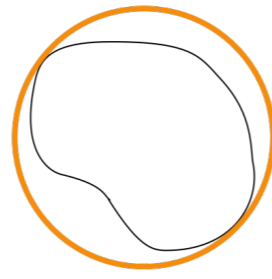
Bounding-volumes



AABB

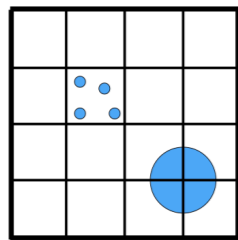


k-DOP

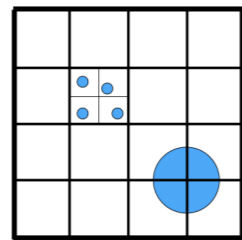


Sphere

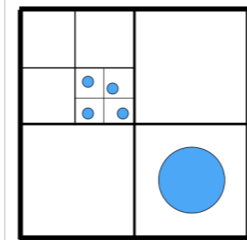
Space partitioning data-structures



Uniform grid



Hierarchical grid

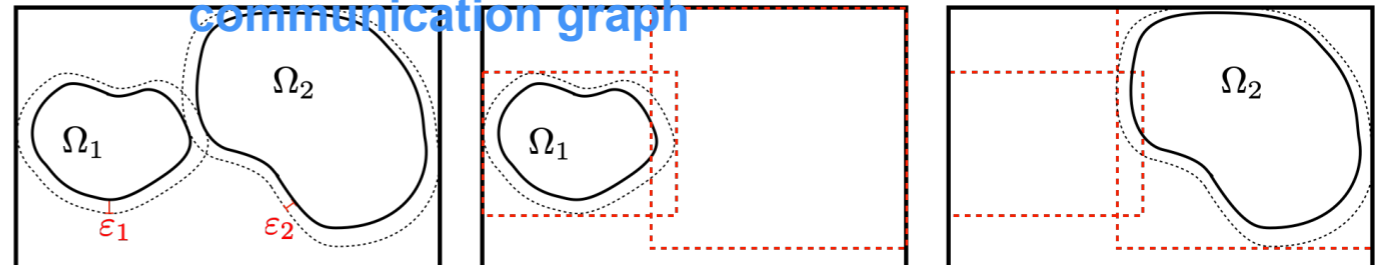


Quad-tree

Parallel tree-search

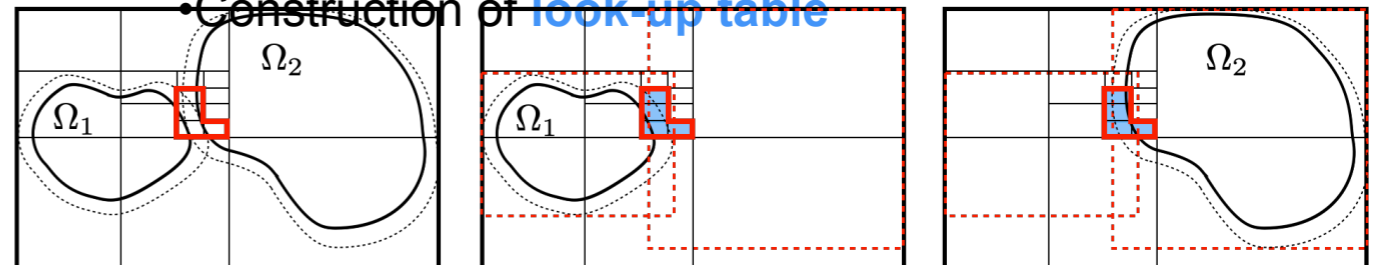
Broad-phase detection

- Computation of local bounding volumes
- **All-to-all** communication
- Construction of **sparse** point-to-point communication graph



Middle-phase detection

- Tree-construction and *asynchronous* point-to-point tree comparison
- Construction of **look-up table**



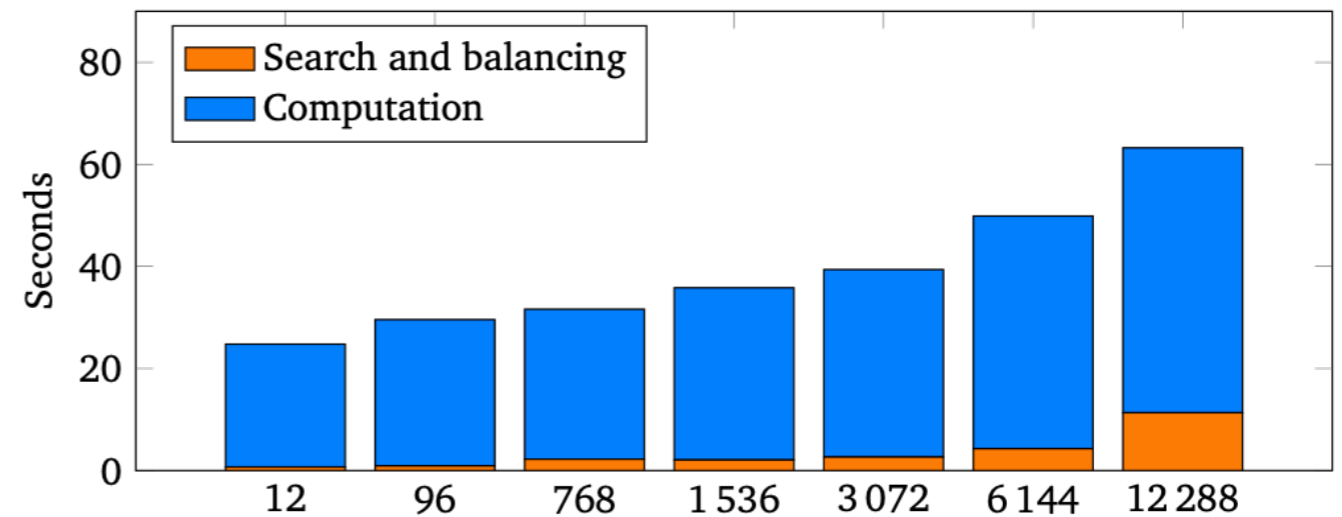
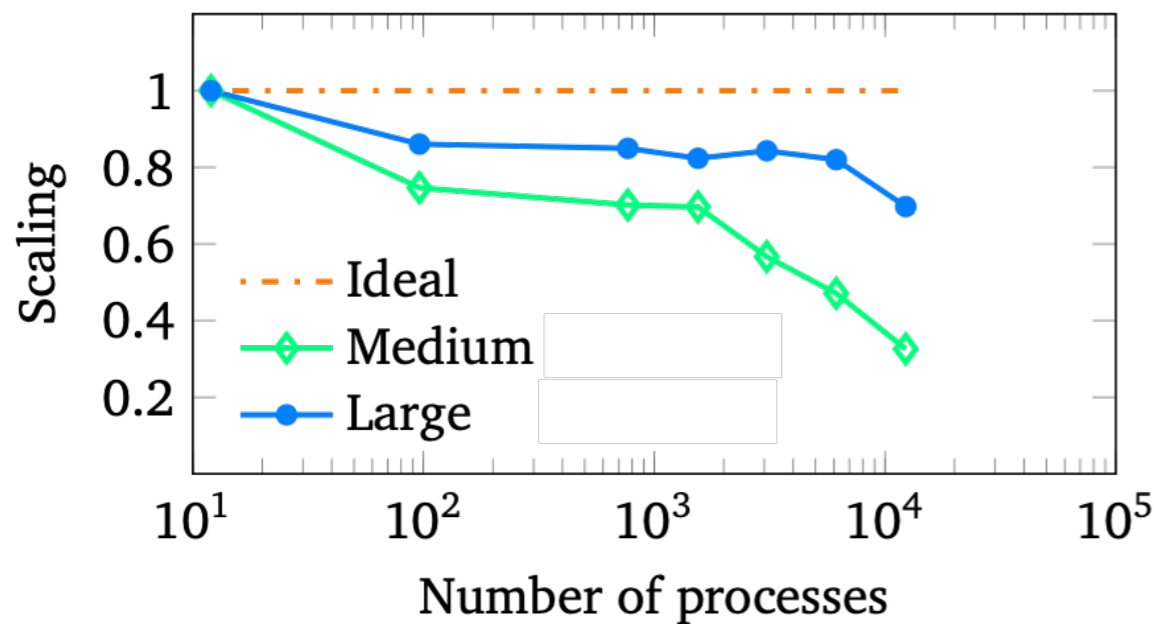
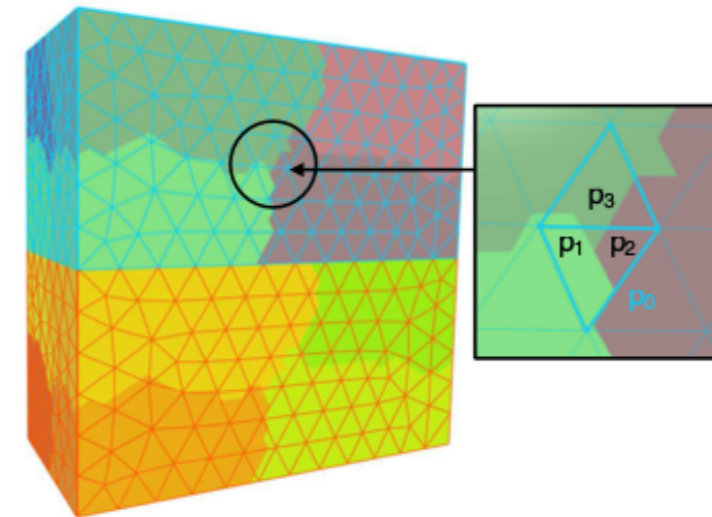
Article: A parallel approach to the variational transfer of discrete fields between arbitrarily distributed unstructured finite element meshes, R. Krause and P. Zulian, SIAM Journal of Scientific Computing 2016

Variational transfer: weak scaling

Experiments:

- **Small** 10 000 elements per process
- **Large** 150 000 elements per process
- Output is **x4** (max 8e9 intersections)

Weak scaling is measured as
(time base experiment)/(time experiment)

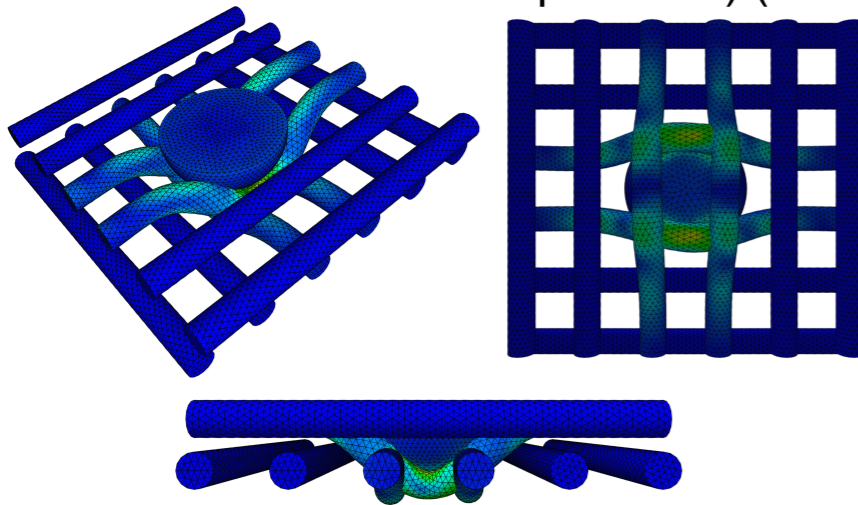
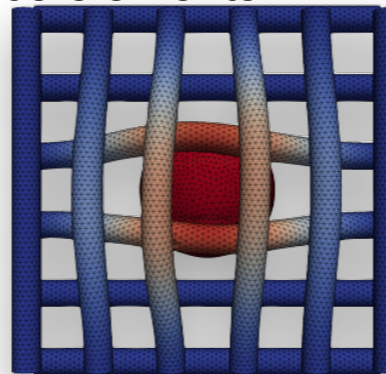


Variational transfer: strong scaling

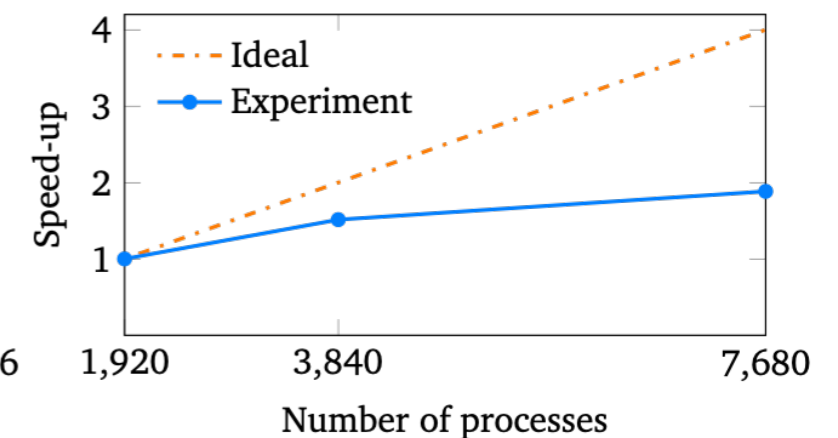
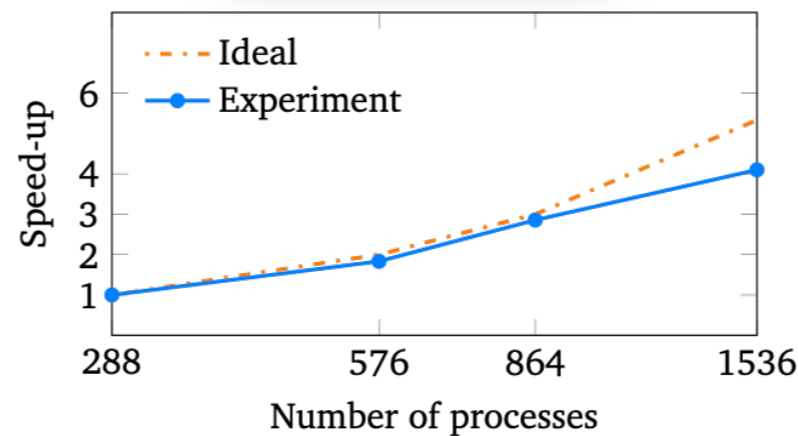
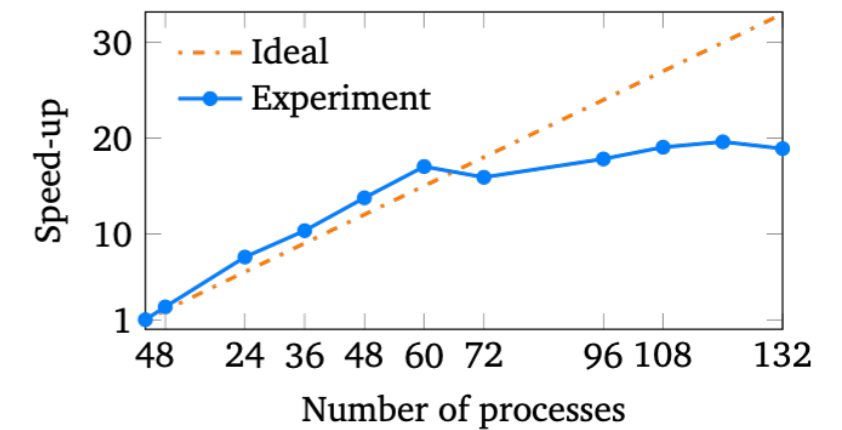
Experiments:

- **Small** 11M elements, 500K surface elements
- **Medium** 700M elements, 8M surface elements
- **Large** 5G elements, 30M surface elements
- Output is $\times 0.1$

Strong scaling is measured as
(time base experiment)/(time experiment)



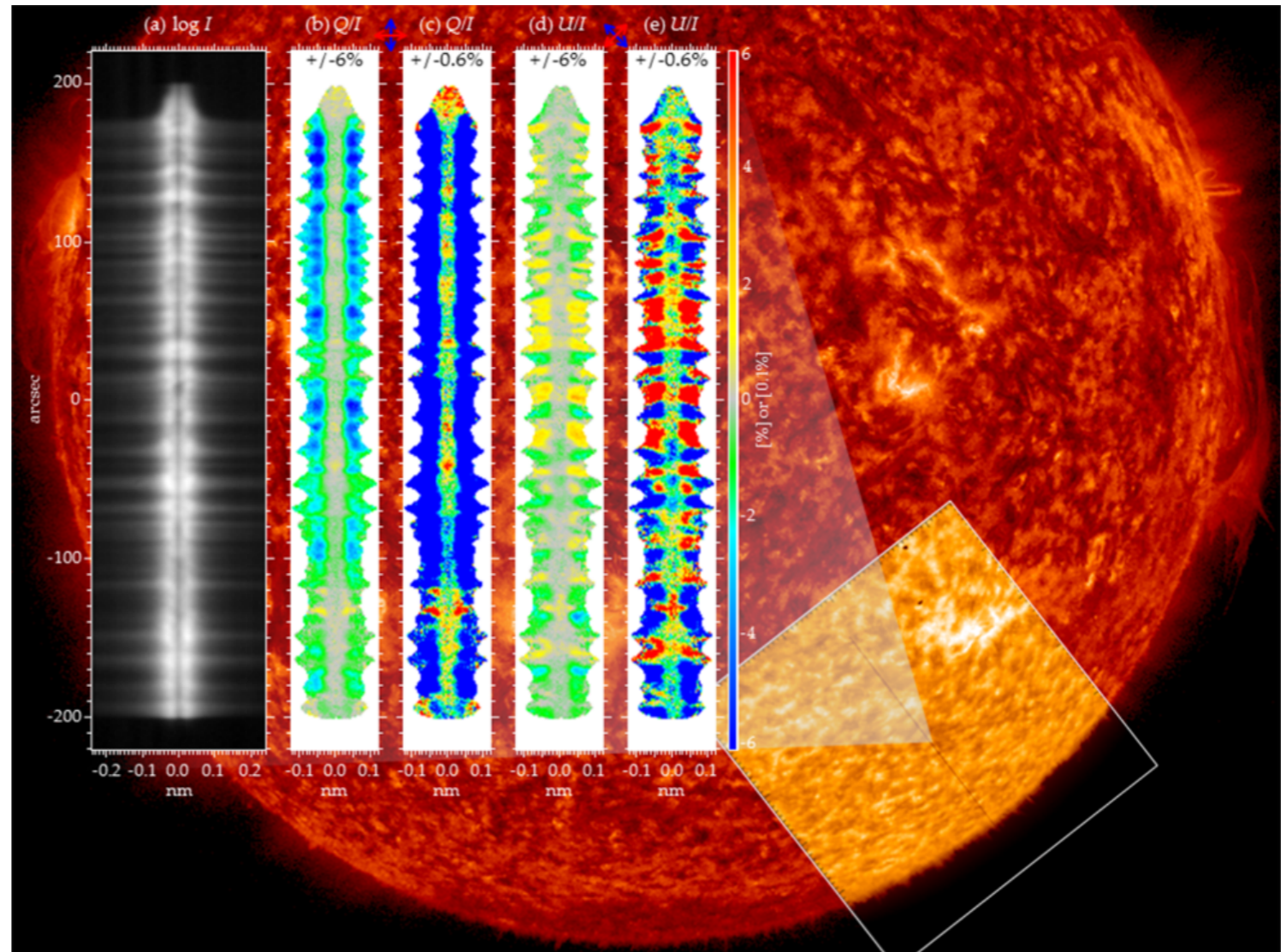
Example simulation



Polarized radiative transfer to understand Sun magnetism

Key problem in solar physics: investigate the magnetism of the outer layers of the solar atmosphere (chromosphere and transition region)

How to do that: by deciphering the information that the magnetic fields on the sun encode in the polarization of solar light



Task: to model the polarization of the solar radiation by *numerically solving the radiative transfer problem for 3D models of the solar atmosphere*

Computational challenge: to solve this problem particular physical processes (partial frequency redistribution (PRD) effects), which strongly affect the polarization of chromospheric spectral lines.

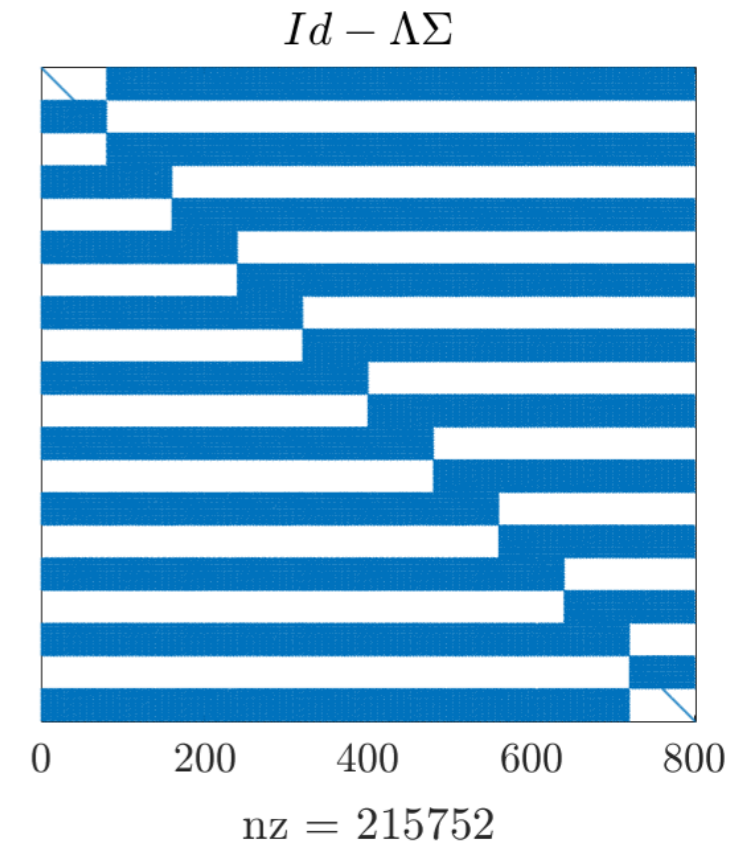
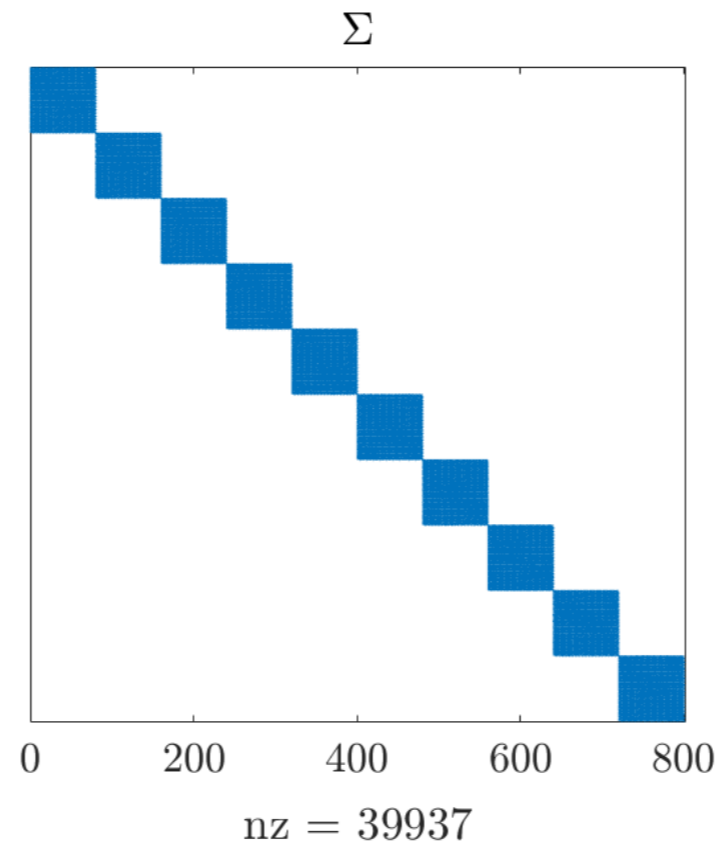
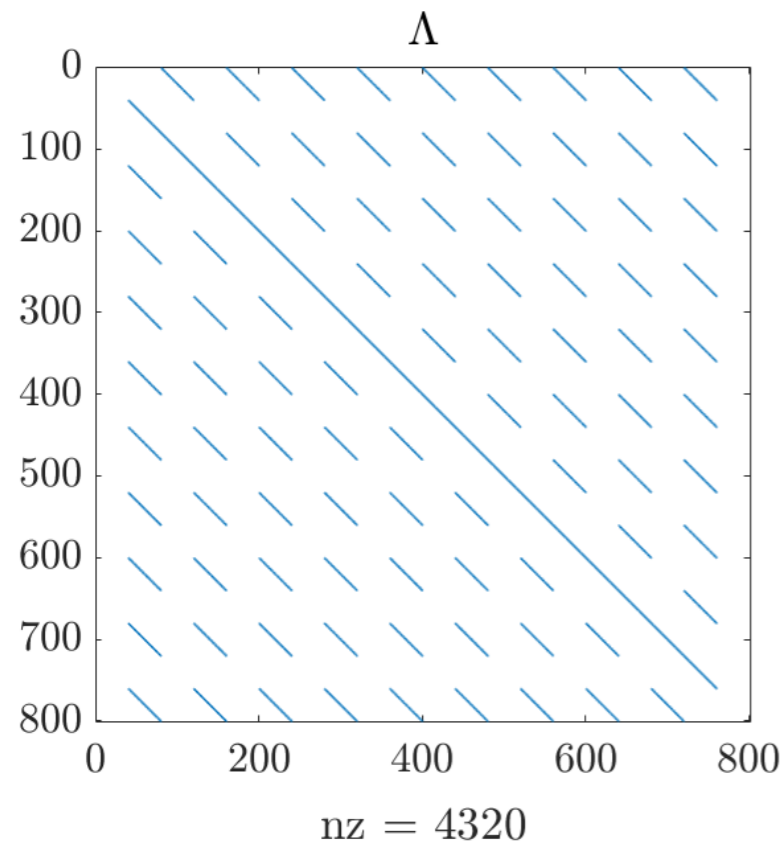
State of the art: for polarized radiation never solved in 3D taking PRD effects into account

RT algebraic formulation

Combining $\mathbf{l} = \Lambda \boldsymbol{\varepsilon} + \mathbf{t}$ and $\boldsymbol{\varepsilon} = \Sigma \mathbf{l} + \boldsymbol{\varepsilon}^{\text{th}}$:

$$(\text{Id} - \Lambda \Sigma) \mathbf{l} = \mathbf{t} + \Lambda \boldsymbol{\varepsilon}^{\text{th}},$$

with RT operator $\text{Id} - \Lambda \Sigma$.



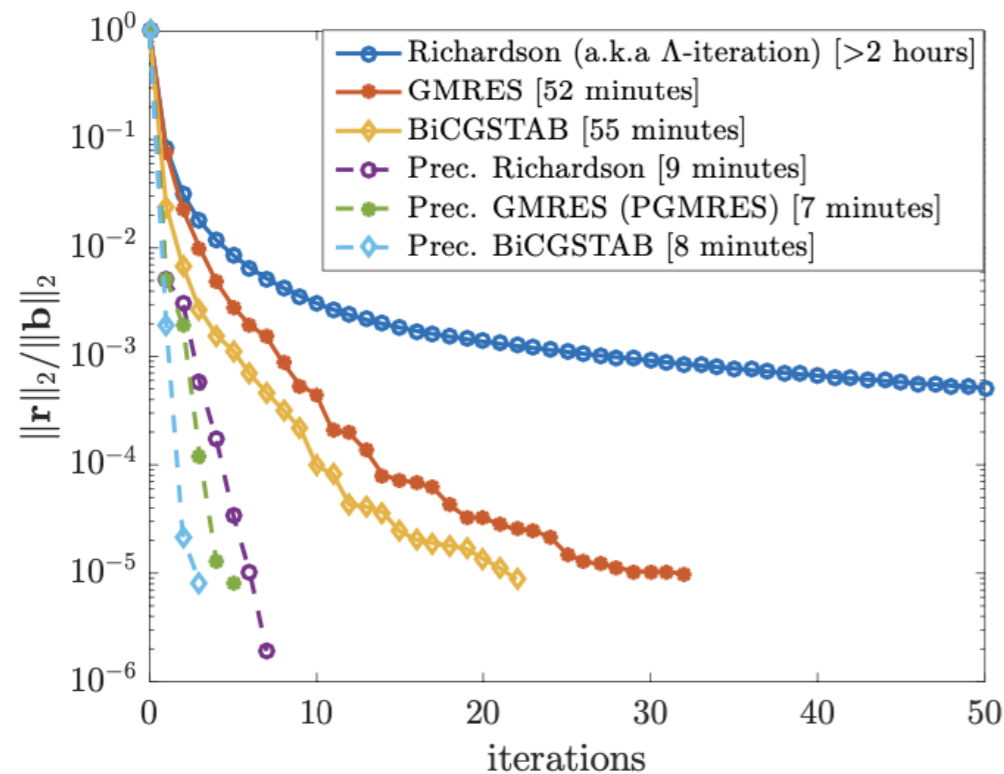
Remarks

- 1 Operators are **matrix-free**
- 2 The cost of applying Λ is negligible w.r.t. the Σ one

Multi-fidelity preconditioner

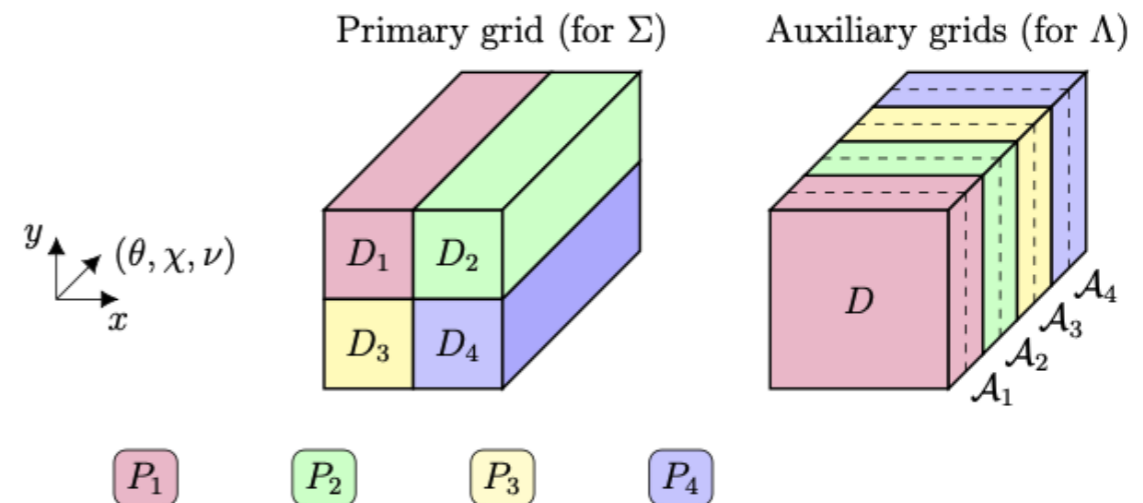
$$P = Id - \Lambda \tilde{\Sigma}$$

- With $\tilde{\Sigma}$ cheap approximation of Σ (CRD)
- Computing P^{-1} action using GMRES



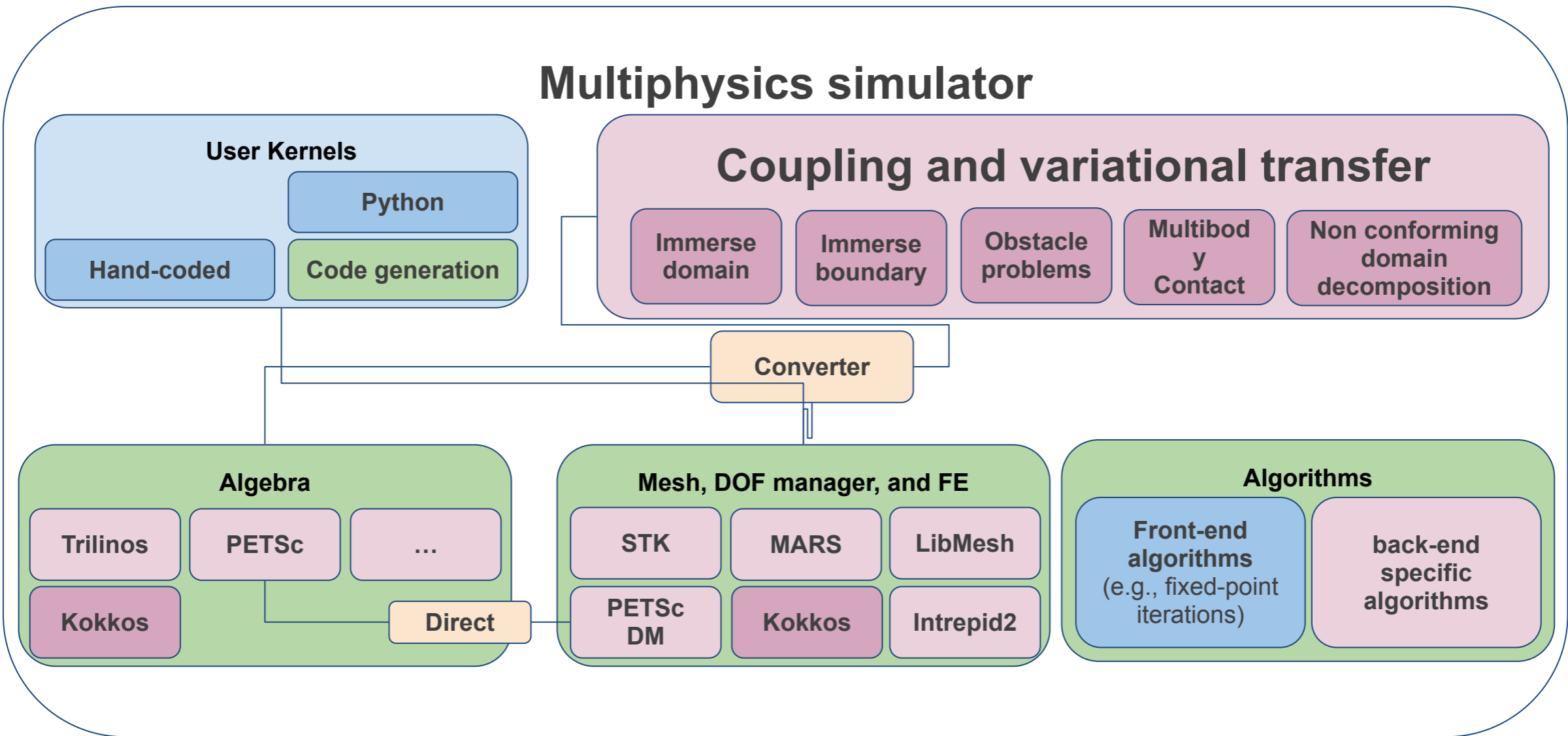
Remarks

- Robust strategy w.r.t. all disc. parameters
- Σ and $\tilde{\Sigma}$ evaluation embarrassingly parallel over N_s
- Λ evaluation embarrassingly parallel over $N_\Omega N_v$



Single call to `MPI_All_to_all()` to exchange data (no ghost layers)

Multiphysics simulator



Legend



Thank you