Fast and scalable finite element algorithms for coupled multiphysics problems and non-matching grids

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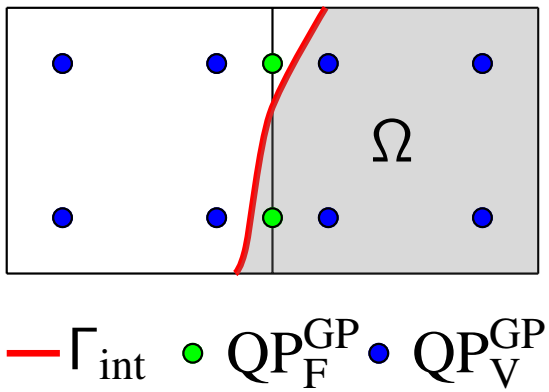
Project overview

- Active in research area of computational fluid dynamics (CFD)
- Project started at my former institute at TUM
- Despite start in 2021, Ph.D. student only getting hired now
- Project now split between UniA and TUM
- My background:
  - Diploma in applied mathematics, Ph.D. in scientific computing, post-doc in computational mechanics
  - Interdisciplinary research, bringing modern mathematical tools to challenging application context with **good utilization of modern hardware**
- Accessed via complex software stack
  - Mathematical abstraction of finite element algorithms by deal.II library (500k lines of C++ code), `github.com/dealii/dealii`
  - Iterative solvers through Trilinos, PETSc, hypre, etc.
  - Large-scale parallelization

One project objective: CutFEM

Selected application of project

- Work on immersed domains by cut finite element methods (CutFEM)
  - Domain boundary implicitly defined by a function (e.g. level set)
  - Computational integrals on **parts** of cells and faces only
  - Typical integration domain defined by implicit function theorem (by R.I. Saye, implemented in deal.II)

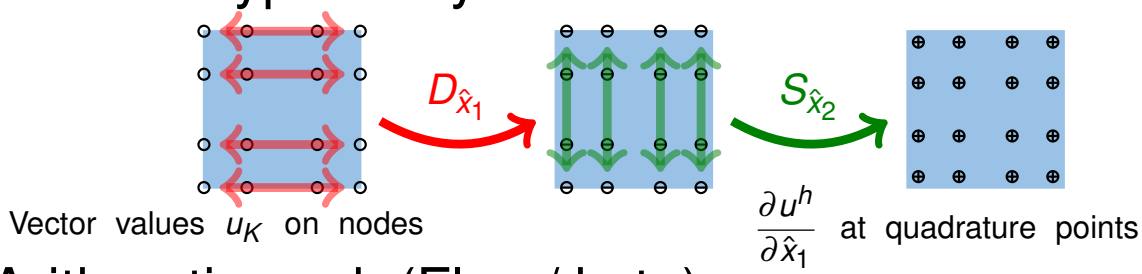


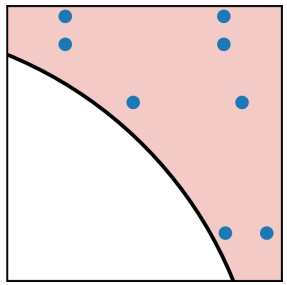
Computational challenge

- Finite element solution must be looked up on arbitrary points on surface or interior of elements
- On each element, must perform transformations between reference coordinates $\hat{\mathbf{x}}$ and real coordinates $\mathbf{x} = \mathbf{F}(\hat{\mathbf{x}})$
- Load balancing is challenging

Research approach: Performance modeling

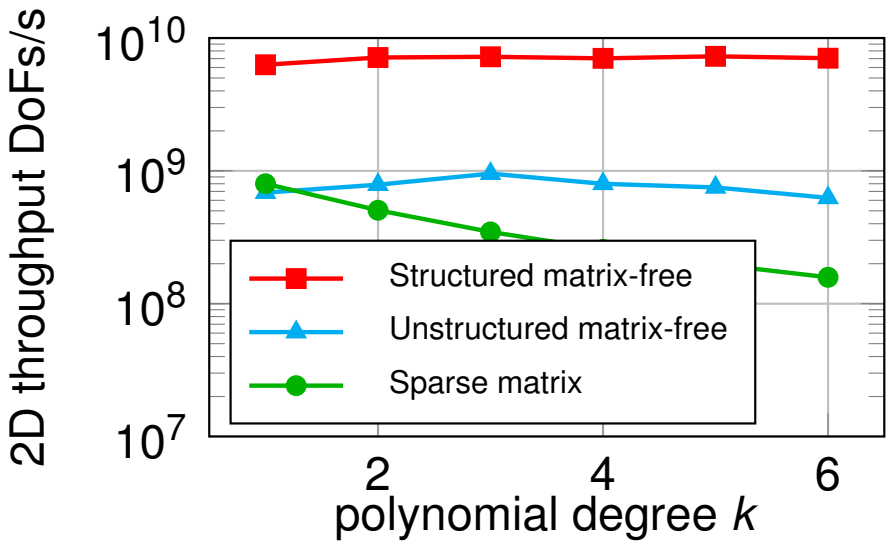
- Roofline-type analysis: Structured vs. unstructured

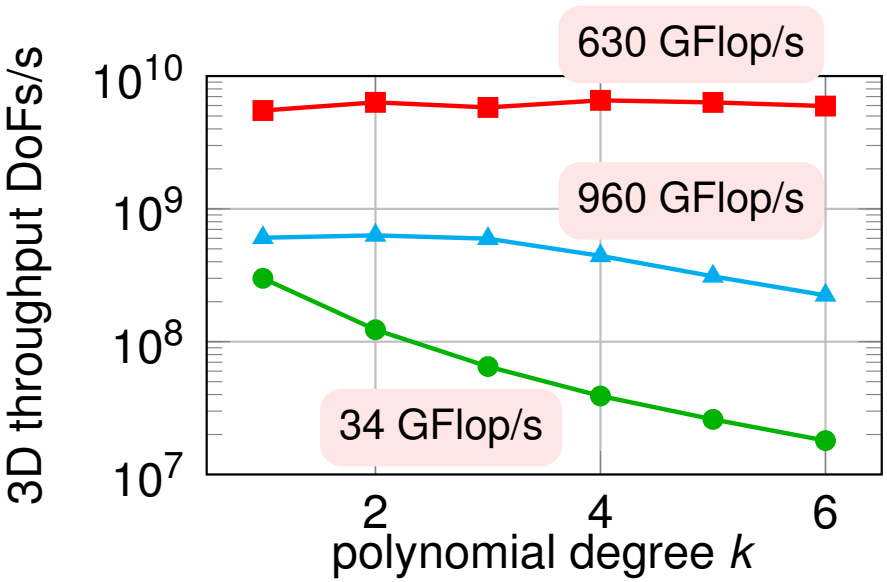




- Arithmetic work (Flop / byte)

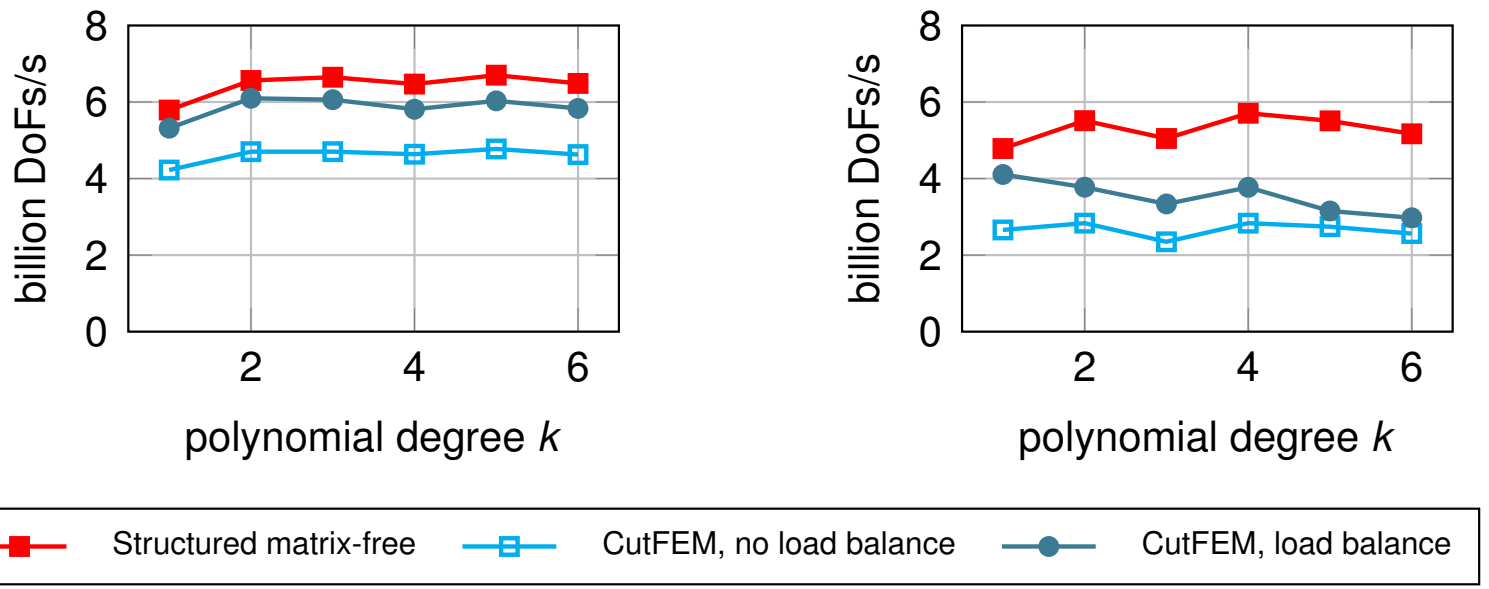
pol. degree p	1	2	3	4	5	6
2D, structured	2.4	2.0	2.4	2.5	2.6	2.7
2D, unstructured	5	13	23	31	39	46
3D, structured	3.5	3.2	3.5	3.7	4.1	4.3
3D, unstructured	12	24	55	96	130	180





Ongoing research

- Roofline model suggests to reduce computations on unstructured case
  - Pre-compute some information on geometric factors
  - Identify re-occurring terms (math)
- Analyze load balancing and communication bottlenecks



- Used on SuperMUC-NG (CPU), Fritz cluster on RRZE @ FAU (CPU)

Possible interactions

- We often work with LIKWID tools and finite-difference-inspired models
  - Translate to FEM context
- LRZ has experience with other tuning tools such as Intel Advisor, MPI bottleneck analysis, etc.
- We combine insights on various levels to produce better implementations
- Hardware access allows us to anticipate future developments
- Currently working on oneAPI port of sample algorithm (LRZ and Intel staff)
- Investigating GPU performance on Alex GPGPU system of RRZE @ FAU