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TWO SCALES ADAPTATION AND SEARCH SPACE RECYCLING FOR ADAPTIVE MULTIPRECONDITIONED FETI

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In a previous work, we developed a new domain decomposition method: Adaptive Multipreconditioned FETI (AMPFETI). AMPFETI is the combination of the dual domain decomposition method FETI and the adaptive multipreconditioned conjugate gradient. AMPFETI is robust enough to solve ill conditioned finite element systems arising from large scale non linear industrial problems. At each iteration, AMPFETI generates as many search directions as there are subdomains in the decomposition. Depending on the result of the adaptive test, these search directions are then kept separatly or gathered. In the case of large and ill-conditioned systems, the memory needed to store all kept search directions may become excessive. This motivated a new version of AMPFETI in which the multipreconditioning is defined at a coarser level: subdomains are grouped in aggregates and each aggregate provide a search direction. It allows a better control off the memory consumption. In this contribution we present a new variant of AMPFETI in which aggregates evolve during the krylov iterations. We also couple AMPFETI with classic deflation techniques and show some new results on real industrial testcases.

HYBRID HIGH-ORDER METHODS FOR DIFFUSION PROBLEMS ON POLYTOPES AND CURVED ELEMENTS

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Originally introduced in [1, 2], Hybrid High-Order (HHO) methods provide a framework for the discretisation of models based on PDEs with features that set it apart from traditional ones; see [4] for a comprehensive introduction. The construction hinges on discrete unknowns that are broken polynomials on the mesh and on its skeleton, from which two key ingredients are devised:

(i) Local reconstructions obtained by solving small, trivially parallel problems inside each element, and conceived so that their composition with the natural interpolator yields a (problem-dependent) projector on local polynomial spaces;

(ii) Stabilisation terms that penalise residuals designed at the element level so as to ensure stability while preserving the approximation properties of the reconstruction.

These ingredients are combined to formulate local contributions, which are then assembled as in standard Finite Element methods. From this construction, several appealing features ensue: the support of polytopal meshes and arbitrary approximation orders in any space dimension; an enhanced compliance with the physics; a reduced computational cost thanks to the compact stencil along with the possibility to locally eliminate a large portion of the unknowns.

In this presentation, focusing on a diffusive model problem, we introduce the basic construction underlying HHO methods on meshes with straight faces and, following [3], point out an extension to curved elements. The key idea, in the latter case, consists in increasing the polynomial degree of the face unknowns according to the so-called effective (geometric) mapping order. A panel of numerical examples including comparisons with Discontinuous Galerkin methods accompanies the exposition.

References

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NONLINEARY PRECONDITIONED FETI METHOD

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We consider the Finite Element approximation of the solution to nonlinear elliptic partial differential equations such as the ones encountered in (quasi)-static mechanics, in transient mechanics with implicit time integration, or in thermal diffusion. Non-overlapping domain decomposition methods (DDM) offer an interesting framework for the distribution of the resolution. We focus on methods allowing independent nonlinear computations on the subdomains, sometimes called "nonlinear relocalization techniques".

Nonlinear counterparts to classical non-overlapping DDM have been proposed: nonlinear primal (Dirichlet) and mixed (Robin) approach [Philippe Cresta, Olivier Allix, Christian Rey, and St phane Guinard. Nonlinear localization strategies for domain decomposition methods: Application to post-buckling analyses. Computer Methods in Applied Mechanics and Engineering, 196(8):1436 1446, 2007], dual approach [Julien Pebrel, Christian Rey, and Pierre Gosselet. A nonlinear dual-domain decomposition method: Application to structural problems with damage. International Journal for Multiscale Computational Engineering, 6(3), 2008], and nonlinear FETI-DP and BDDC [Axel Klawonn, Martin Lanser, and Oliver Rheinbach. Nonlinear FETI-DP and BDDC Methods. SIAM Journal on Scientific Computing, 36(2):A737 A765, 2014]. The latter methods were improved and assessed at a large scale in [Axel Klawonn, Martin Lanser, Oliver Rheinbach, and Matthias Uran. Nonlinear FETI-DP and BDDC methods: A unified framework and parallel results. SIAM J. Sci. Comput., 39(6):C417 C451, 2017]. A global framework for primal/dual/mixed approaches was also proposed [Camille Negrello, Pierre Gosselet, Christian Rey, and Julien Pebrel. Substructured formulations of nonlinear structure problems – influence of the interface condition. International Journal for Numerical Methods in Engineering, 2016] and the impedance of the mixed approach was improved [Camille Negrello, Pierre Gosselet, and Christian Rey. A new impedance accounting for short and long range effects in mixed substructured formulations of nonlinear problems. International Journal for Numerical Methods in Engineering, 2017].

Our objective is to double the intensity of the local independent nonlinear computations by modifying the condensed problem to be solved. The method can be interpreted as proposing a nonlinear preconditioner [Peter R Brune, Matthew G Knepley, Barry F Smith, and Xuemin Tu. Composing scalable nonlinear algebraic solvers. SIAM Review, 57(4):535 565, 2015] to the nonlinear DDM.

It appears that this idea applies particularly easily to the dual approach, under an hypothesis equivalent to infinitesimal strain in mechanics. When applying a Newton algorithm to this nonlinear preconditioned condensed system, one alternates a sequence of two independent nonlinear local solves (one Neumann problem and one Dirichlet problem separated by one all-neighbor communication) and an interface tangent solve which exactly has the structure of a linear preconditioned FETI problem. Academic assessments show that the sequence of two local nonlinear solves can reduce the need of global Newton iterations and thus the number of calls to the communication-demanding Krylov solver.

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THE FROSCH PACKAGE IN CARDIOVASCULAR SIMULATIONS

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FROSch (Fast and Robust Overlapping Schwarz), a framework for overlapping Schwarz preconditioners, has recently been integrated into Trilinos as part of the package ShyLU. It contains scalable preconditioners that are robust for a wide class of problems, e.g., from solid or fluid mechanics, and can be constructed in an algebraic way. In particular, the preconditioners can be constructed from the fully assembled matrix without an additional coarse triangulation, even for unstructured domain decompositions. Additional information about the geometry or the null space of the operator can further improve the convergence and robustness of the solvers.

This talk gives an overview of the FROSch code, its features, and user-interface and shows the parallel scalability and robustness of the solvers for different problems. In particular, the focus of this talk lies on the application of FROSch in large-scale simulations of blood flow in arteries and the deformation of arterial walls.

Based on joint work with Christian Hochmuth, Sivasankaran Rajamanickam, and Friederike Röver.

ON THE INTEREST OF HIGH MEMORY BANDWIDTH ARCHITECTURES FOR PDE DISCRETIZATIONS WITH COMPACT SUPPORT

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The arithmetic intensity of PDE discretization schemes with compact support, in particular on unstructured meshes, is so low that on current architures these schemes are limited by the available bandwidth more than by the computational power. Over the last few years, a small number of high bandwidth memory (HBM) systems have become available. We will present performance results on one of these architectures, the NEC vector engine SX-Aurora Tsubasa, and compare it to the performance prediction of the roofline model.

DOMAIN DECOMPOSITION IN COMPUTATIONAL HOMOGENIZATION WITH MILLION-WAY PARALLELISM

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The computational simulation of modern high-strength steel materials with micro structure is still a challenge. As a computational homogenization approach we consider the FE^2 method combined with efficient parallel domain decomposition methods of FETI-DP type. In the FE^2 approach, in each Gauss integration point of the macroscopic problem, a microscopic problem on a representative volume element (RVE) is solved. The microscopic problems are only coupled through the macroscopic level and can be solved all in parallel. Each of these microscopic problems itself will be solved using a parallel FETI-DP domain decomposition method. This approach is implemented in PETSc and uses efficient solver packages including BoomerAMG, MUMPS, and UMFPACK, resulting in the parallel computational homogenization software FE2TI. We present weak scalability results obtained using several hundred thousands of cores and more than a million MPI ranks.

ON FAST ITERATIVE SOLVERS FOR PROBLEMS IN STRUCTURAL MECHANICS

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The prestressed concrete structure of civil engineering buildings can be modeled as a problem in linear elasticity for which one-, two- and three-dimensional finite elements are coupled by multi-point constraints. Multi-point constraints describe linear relationships between degrees of freedom and are introduced in the discrete system. Enforcing these constraints by Lagrange multipliers results in a symmetric indefinite matrix with a 2x2 block structure. In practice, these systems are very difficult to solve since they become quickly too large for direct solvers and common iterative methods work only poorly on them.

In this talk, we present a new iterative solver that is based on the Golub-Kahan bidiagonalization (GKB) method, which has been widely used in solving least-squares problems and in the computation of the singular value decomposition of rectangular matrices. The algorithm is applied to matrices that are generated by code_aster, an open-source finite element software developed at the French electricity utility company EDF. We show that the GKB method has excellent convergence properties for this problem class and that, for a good choice of some parameter, the number of iterations depends only weakly on the discretization size. This generalized GKB algorithm has also been implemented in PETSc and we present its scalability on practical problems. In particular, as a linear system of the size of the (1,1)-block has to be solved in each iteration of the GKB method, we compare the performance of direct and iterative methods for the solution of this inner linear system.

ON AN EFFICIENT PARALLEL IMPLEMENTATION OF ADAPTIVE FETI-DP WITH LOAD BALANCING

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Domain decomposition methods such as FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) and BDDC (Balancing Domain Decomposition by Constraints) are highly scalable parallel solvers for large sparse systems obtained from the discretization of partial differential equations (PDEs).

However, the convergence behavior of FETI-DP and BDDC methods with a standard coarse space highly depends on the parameters of the underlying PDE. The convergence rate of both methods can deteriorate significantly if composite materials are considered. In such cases, problem-dependent (or adaptive) coarse spaces offer a remedy. In adaptive methods, difficulties arisen from highly heterogeneous materials are detected automatically by solving local generalized eigenvalue problems and an adaptive coarse space is set up. These methods are thus characterized by great robustness.

Though, for an efficient parallel implementation, different issues such as load imbalances and the solution of unnecessary eigenvalue problems have to be avoided and the eigenvalue solver has to be optimized to reduce the computational overhead in the set up phase. We will present details of the set up of the adaptive method to implement the coarse space enrichment efficiently in a parallel context.

We will present weak and strong scaling results to show the good parallel scalability of our method.

SURROGATE POLYNOMIALS IN MATRIX-FREE APPROACHES FOR LOW-ORDER FEM

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It has been noted for some time that the classical finite element procedure of discretising the PDE problem, assembling the global system matrix, storing it in some sparse matrix format and employing the latter in the solution process of the associated linear system is posing a bottleneck for performance in the context of large-scale applications. This is due to the huge disparity in the time required to perform floating point operations on current architectures and the time required for transferring the required operands through the memory system. Implementations following this paradigm are typically, what is denoted as, memory bound and, thus, only reach a meagre percentage of the theoretical peak performance of the systems.

Hence, matrix-free approaches, which do not explicitly store the system matrix, but facilitate the evaluation of a matrix-vector-product (MVP), are attracting considerable attention, especially in the light of upcoming exascale supercomputers. Computing the cell-wise MVP contributions by fusing them with the local integral evaluations has proven very successful for higher-order FE discretisations.

We are going to present a different idea which is based on the use of polynomial approximations of entries of local element matrices. This surrogate matrix methodology can provide significant performance advantages in the case of locally structured meshes. This approach can be seen as a variational crime and can be analysed accordingly. In our presentation we will mostly focus on numerical convergence and scaling results for problems ranging from the variable coefficient Poisson to the generalised Stokes problem of geodynamic convection demonstrating the applicability and efficiency of this approach. Our largest simulation, used to investigate the dynamic topography in models with lateral viscosity variations, employs a global mesh resolution of 1.5 km resulting in a trillion ($\mathcal{O}(10^{12})$) degrees of freedom.

MULTIGRID PRECONDITIONERS FOR FINITE ELEMENT AND DG DISCRETISATIONS: APPLICATIONS IN GEOPHYSICAL FLUID DYNAMICS

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Numerical weather- and climate- prediction models rely on algorithmically optimal time-integrators and fast linear solvers. Modern codes have to make efficient use of massively parallel computer hardware and deliver forecasts under very tight time constraints. Semi-implicit integrators allow the separate treatment of fast and slow atmospheric waves and permit larger model timesteps. However, they require the repeated solution of very large, ill-conditioned sparse systems of equations which is only possible with algorithms such as the multigrid method. In operational configurations, systems with $10^9 - 10^{12}$ unknowns have to be solved within in a few seconds.

Advanced discretisations, such as mimetic Finite Elements and Discontinuous Galerkin (DG) approaches are currently implemented for next-generation operational models. This includes, for example, the UK Met Office's forecast model "LFRic" and the "NUMA" code developed in the US. Those discretisations offer flexibility on non-trivial grids, allow the exact conservation of physical quantities and can increase data-locality. By using sum-factorisation techniques, higher-order discretisations also permit the efficient utilisation of modern chip architectures with a poor bandwidth-to-FLOP ratio. The design of good multigrid solvers is, however, very challenging since the traditional Schur-complement reduction to a system in pressure space is hampered by non-diagonal mass-matrices and artificial diffusion terms.

In this talk I will discuss the implementation of bespoke multigrid solvers in operational weather- and climate models and describe some recent progress on solvers for hybridised DG methods. In addition to discussing the design of the algorithms, I will comment on the implementation and performance portability: being able to run and maintain the model on different architectures and massively parallel supercomputers is an increasingly important aspect.

CROSSBREADS—IDEAS BEHIND ALMOST MATRIX-FREE, ALGEBRAIC-GEOMETRIC MULTIGRID SOLVERS

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Geometric multigrid solvers with operator rediscretisation are the method of choice to solve large-scale elliptic problems. They have a small memory footprint, we can implement them in a streaming fashion, there is not much administrative overhead if we combine them with tree-based adaptive meshes, and so forth. There's only one problem: they tend not to work as soon as we tackle non-trivial problems with anisotropic operators, jumping material parameters or convection terms. We present a merger of geometric multigrid relying on spacetrees with the algebraic BoxMG technique. A combination with FAC/HTMG allows us to support arbitrary dynamic adaptivity straightforwardly, while pipelining allows us to write single-touch implementations. On-the-fly compression of the data finally yields an algebraic solver with a memory footprint close to its geometric counterpart.