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Factorizing the factorization – a spectral-element solver for elliptic equations with linear operation count

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ABSTRACT

The paper proposes a novel factorization technique for static condensation of a spectral-element discretization matrix that yields a linear operation count of just $13N$ multiplications for the residual evaluation, where N is the total number of unknowns. In comparison to previous work it saves a factor larger than 3 and outpaces unfactored variants for all polynomial degrees. Using the new technique as a building block for a preconditioned conjugate gradient method yields linear scaling of the runtime with N which is demonstrated for polynomial degrees from 2 to 32. This makes the spectral-element method cost effective even for low polynomial degrees. Moreover, the dependence of the iterative solution on the element aspect ratio is addressed, showing only a slight increase in the number of iterations for aspect ratios up to 128. Hence, the solver is very robust for practical applications.

1. Introduction

While spectral Fourier methods [1] provide the optimum efficiency for the high accuracy computation of regular solutions due to the spectral convergence and the availability of fast transformations, they require periodic boundary conditions or some particular treatment, such as damping zones, for more complex cases. Spectral methods based on more general orthogonal polynomials are also employed for flow simulations [2], but are often restricted to regular solutions and a reduced set of boundary conditions as well. Other high-order schemes like the discontinuous Galerkin (DG) methods or the spectral-element methods (SEM) have been conceived for geometrical flexibility and the possibility to adjust the order of approximation. For these (and other) reasons, the latter have been receiving vital interest from the community during the last years. Yet, fast solvers for these methods are still a matter of research.

As with high-order methods the number of degrees of freedom inside an element scales with the polynomial degree to the power of three, ways to reduce the algebraic problem size are sought. The static condensation method is often used to this end. For instance the first work on SEM in [3] already employs it, as do more recent ones [4,5]. Other applications of static condensation include the explicit solution for cuboidal geometries [6], p-multigrid techniques for rectangular geometries [7] and the application as preconditioner for a DG scheme [8].

The algorithms in the cited references benefit from the static condensation with spectacular increases in performance. However, they all share one downside: When increasing the polynomial degree, the operation count scales super-linearly

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with the number of degrees of freedom, so that the method becomes less and less efficient with higher and higher polynomial degrees. To remain efficient at high polynomial degrees, linear complexity is required throughout the entire solver, from the operator execution, to the preconditioner, to the remaining operations inside an iteration.

As the implicit treatment of diffusion terms and pressure-velocity coupling in solvers for incompressible fluid flow often reduce to a Helmholtz equation, the goal of this article is to provide a Helmholtz solver with linear scaling. It extends earlier works of the authors in [9] and [10], where preliminary variants of the condensed Helmholtz operator with linear operation count were proposed. While these variants resulted in linear execution times of the iterations, they outperformed unfactorized versions implemented via dense matrix–matrix multiplications only for polynomial degrees $p > 10$. Current simulations, however, tend to use lower polynomial degrees [11,5,12] so that with these methods a gain might not be achieved. The present paper proposes an efficient static condensation method for a spectral-element discretization using cuboidal elements, outperforming matrix–matrix multiplications down to a polynomial degree of $p = 2$. Similar to the work in many of the cited references, the development is performed for a Cartesian discretization here.

The paper is laid out as follows: Section 2 focuses on tensor-product matrices as a necessary prerequisite and the third section on the spectral-element method. Section 4 recapitulates the static condensation while the fifth section recalls operators from [9]. Section 6, finally, puts these elements together and proposes the new method. In Section 7 and 8, the efficiency of the new operators and solvers is quantitatively assessed with suitable test cases.

2. Tensor-product matrices

Many partial differential equations exhibit a separable substructure [13], i.e. the differential operator can be decomposed into smaller operators acting in single coordinate directions only. This allows for further analysis of the operator and the resulting system matrices. Indeed, it is the basic approach to lower the operation count here, as illustrated by the following very simple example. Assume that a two-dimensional problem is discretized using a spectral method with n degrees of freedom in each direction such that the vector of discrete unknowns is $\mathbf{v} \in \mathbb{R}^{n^2}$. The system matrix $\mathbf{C} \in \mathbb{R}^{n^2,n^2}$ is dense, so that its straightforward application requires n^4 multiplications. If it is a tensor-product matrix, however, its application can be reformulated as

$$\mathbf{Cv} = (\mathbf{B} \otimes \mathbf{A})\,\mathbf{v} = (\mathbf{B} \otimes \mathbf{I})\,(\mathbf{I} \otimes \mathbf{A})\,\mathbf{v} \tag{1}$$

with $\mathbf{I} \in \mathbb{R}^{n,n}$ being the identity matrix, $\mathbf{A} \in \mathbb{R}^{n,n}$ the operator in the first direction and $\mathbf{B} \in \mathbb{R}^{n,n}$ the operator in the second one. The consecutive application of $\mathbf{A}$ and $\mathbf{B}$ then requires only $2n^3$ multiplications. In general, tensor products of dimension d require only dn^{d+1} multiplications compared to n^{2d} for the application of the whole matrix.

Tensor-product matrices possess additional properties that allow for factorization techniques. E.g., the multiplication of two tensor-product matrices is reducible to the multiplication of the respective submatrices

$$(\mathbf{A} \otimes \mathbf{C})\,(\mathbf{B} \otimes \mathbf{D}) = (\mathbf{AB}) \otimes (\mathbf{CD}) \quad . \tag{2}$$

Also, transpose and inverse can be reformulated

$$(\mathbf{A} \otimes \mathbf{B})^T = \mathbf{A}^T \otimes \mathbf{B}^T \tag{3}$$

$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1} \quad . \tag{4}$$

Further properties and applications of tensor-product matrices are presented in [13] and [14].

3. The spectral-element method with cuboidal elements

The continuous Helmholtz problems in a domain Ω reads

$$\lambda u - \Delta u = f \quad , \tag{5}$$

where u is the variable to solve for, $\lambda \geq 0$ is a real constant parameter, Δ the Laplace operator and f the right-hand side. This equation was first formulated in the field of acoustic research with $\lambda < 0$. Nonetheless, the case $\lambda \geq 0$ is commonly referred to as Helmholtz equation in the fluid dynamics community.

Decomposing the domain into n_{e} elements Ω_e, the spectral-element method leads to the discrete equation system

$$\mathbf{R}\mathbf{H}_{\mathrm{L}}\mathbf{R}^T\mathbf{u}_{\mathrm{G}} = \mathbf{R}\mathbf{F}_{\mathrm{L}} \quad , \tag{6}$$

where $\mathbf{u}_{\mathrm{G}}$ is the solution vector, $\mathbf{F}_{\mathrm{L}}$ is the discretized right-hand side, $\mathbf{R}$ gathers the contributions from the elements, and its transpose $\mathbf{R}^T$ scatters the global degrees of freedom to those local to the elements [14,15]. The local Helmholtz operator $\mathbf{H}_{\mathrm{L}}$ is a block-diagonal matrix consisting of the element Helmholtz operators $\mathbf{H}_e$.

This paper only considers the case of cuboidal elements. A three-dimensional tensor-product basis is utilized in each element, allowing the standard element basis functions ϕ_{ijk} to be decomposed into three one-dimensional basis functions such that [14]