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Finite Difference preconditioning for compact scheme discretizations of the Poisson equation with variable coefficients

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5 Abstract

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The finite difference preconditioning for higher-order compact scheme discretizations of non separable Poisson's equation is investigated. An eigenvalue analysis of a one-dimensional problem is detailed for compact schemes up to the tenth-order. The analysis concludes that the spectrum is bounded irrespective of the mesh size and the continuous variable coefficient. Hence, combined to a multigrid method, the preconditioned Richardson method shows a convergence rate which is independent from the mesh size and the variable coefficient. Several numerical experiments, including the simulation of a flow with large density variations, confirm that the spectrum of the preconditioned operator remains bounded.

6 Keywords: Compact schemes, Poisson's equation, preconditioned Richardson method

7 1. Introduction

The accurate numerical solution of the Poisson's equation is often required in the modelling of heat and mass transfer, in the presence of chemical reactions, in several scientific and engineering applications. The Poisson's equation may have constant or variable coefficients depending on the complexity of the problem. Accuracy and computational speed of the numerical solver can be improved by employing higher-order discretization within the framework of parallel methods. The development of such discretization and parallel methods for variable-coefficient Poisson's equation remains a challenge. In this work, a second-order

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¹⁵ finite-difference preconditioning method for higher-order compact schemes to solve the Pois¹⁶ son's equation is developed and assessed for accuracy and computational performance.

One of the straightforward and popular methods to write a discretization of the variable coefficient Poisson equation is the common finite differences, elements or volumes. The resulting discrete Poisson operator is built on a *local* computational stencil and thus can benefit from efficient direct or iterative linear solvers at the cutting edge of the high performance computing [1–3] which permits to compute accurate solutions on fine grids. A recent comparative study of several Poisson solvers in an unit cube has been released by Gholami et al. [4].

Another way to get accurate solution while limiting the number of degrees of freedom is 24 to use higher-order discretizations. Spectral methods are these higher-order discretizations 25 which exhibit an exponential decrease of the numerical error for sufficient regular solutions 26 [5]. This strong property naturally leads authors to consider this discretization when com-27 puting accurate solution of benchmark problems [6]. Unlike lower-order discretizations, the 28 *global* approximation of spectral methods introduces some specific difficulties: spurious oscil-29 lations due to a loss of local regularity conditions [7], large parallel communications inherent 30 to FFT [8], and bad conditioning of discrete operators [5]. Orszag [9] proposed to use 31 Finite-Difference preconditioning to achieve spectral accuracy with the Fourier spectral dis-32 cretization. Haldenwang et al. [10] discussed this approach regarding the Chebyshev spectral 33 approximation. In both works, the theoretical analysis relies on the evaluation of the lowest 34 and highest eigenvalues of the preconditioned discrete operator in the one-dimensional Pois-35 son equation. In addition to the derivation of the convergence rate bound $\pi^2/4$, Haldenwang 36 et al. [10] has shown that the convergence rate is not sensitive to the boundary conditions and 37 to the dimensionality of the problem. Always based on one-dimensional analysis Labrosse 38 and Redondo [11] has presented a way to design an optimal lower-order preconditioner for 39 the Chebyshev discretization of the Poisson 1d problem with a constant coefficient. 40

41 Other popular higher-order discretizations exist, such as the Higher-Order Compact 42 Schemes.These Schemes are a set of higher-order finite differences achieving higher-order

accuracy on a small computational stencil [12–14]. One way to write such schemes is based 43 on the substitution of the higher derivatives occurring in the central finite difference trun-44 cation error with the second-order finite difference approximation. This approach has led to 45 the definition of the Mehrstellen scheme [12]. A large amount of works follows this approach 46 as illustrated by the non-exhaustive selected papers [15-17]. One of the advantages of pro-47 ceeding in this way is that the resulting schemes lead to a sparse linear system irrespective 48 to the problem of dimensionality, or to more general equations like convection/diffusion [18]. 49 Moreover, efficient iterative linear solvers like multigrid methods can benefit from the *local* 50 computational stencil [17]. However, some limits may be outlined. First, the derivation of 51 such schemes can be a tricky problem when non-uniform meshes or staggered grids have to 52 be considered. Then, the derivation of such Mehrstellen-like schemes for the conservative 53 formulation of a non-separable Poisson equation seems to remain an open issue. This con-54 servative formulation is still widely used to achieve conservation properties as for instance 55 in computational fluid dynamics in order to enforce the divergence of the velocity. 56

Another way to derive HOCS discretization for Poisson's equation is to write the problem 57 in a tensorial form and then to write down the discretization in each direction [13]. This 58 approach allows to consider the Poisson's equation on staggered grids [19], or to involve 59 variable coefficients [20]. One of the advantages of the one-dimensional HOCS is that the 60 higher-order accuracy is achieved by solving tridiagonal or pentadiagonal linear systems. 61 This former operation is performed with a linear algorithm complexity, even in parallel ar-62 chitecture [19]. The drawback is, however, that the resulting discrete Poisson operator is 63 no longer sparse. The diagonalization method can be considered to compute solutions for 64 this dense linear system [10]. Alternatively, iterative methods using a matrix free implemen-65 tation can be examined as long as the evaluation of the residual for the Poisson equation 66 is performed with a linear complexity algorithm. But, the bad condition number inherent 67 to the scheme accuracy needs to be reduced by using a specific preconditioner [21]. Abide 68 and Zeghmati [19] showed that a common second-order finite difference preconditioning for 69 the fourth-order compact scheme discretization of the two-dimensional constant coefficient 70

⁷¹ Poisson's equation allows to bound the spectral radius independently to the mesh size.

The case of the non-separable Poisson's equation is approached by several authors with 72 methods similar to the defect correction [22]. The defect correction method introduces a 73 simplified discrete operator, like lower-order discretization and/or constant coefficient, to 74 determine successive corrections of the residual computed with the variable coefficient and 75 eventually using high-order discretizations. This approach is investigated within the frame-76 work of the HOCS discretization of the constant coefficient Poisson equation on a staggered 77 grid [19]. Nicoud [23] introduced a FD preconditioning based on a constant averaged co-78 efficient in the periodic directions to use a FFT-based Fast Poisson Solver. Within the 79 framework of two-phase flows, Dodd and Ferrante [24] investigated a splitting, similar to 80 the first step of the defect correction with a time-extrapolated initial guess for the pressure 81 variable. This procedure is discussed and extended to HOCS discretizations in the context 82 of the simulation of reactive flows based on the low Mach number approximation [25]. The 83 deferred correction is also the strategy considered by Knikker [20] to tackle solutions of the 84 HOCS discretization of Poisson's equation. It is worth mentioning that regardless the dis-85 cretization scheme, the defect correction using a preconditioner based on an approximate 86 coefficient constant Poisson's equation has a convergence rate independent of the mesh-size, 87 but dependent on the bound of the variable coefficients [26]. 88

The present review outlines that the lower-order preconditioning of the spectral dis-89 cretization allows us to design iterative solvers that have a convergence rate independent of 90 the mesh size [10]. A similar analysis for HOCS discretization established a similar result [19] 91 in the case of constant coefficient Poisson's equation. For the variable coefficient Poisson's 92 equation, the literature misses the analysis and the discussion of a such finite-difference pre-93 conditioning for HOCS discretizations. This is addressed by carrying out the computation of 94 the condition number for the preconditioned Richardson iterative solver. The findings of this 95 analysis are verified against several manufactured problems. The simulation flows involving 96 large density gradients are also performed to verify and demonstrate the reliability of the 97 lower-order finite difference preconditioning. 98

The next section presents the HOCS discretization of a non-separable Poisson's equation 100 written in a conservative form and defined on a staggered grid. The exact derivation of the 101 convergence rate for the Richardson method is established in the one-dimensional case for 102 the constant coefficient Poisson's equation. In the case of the variable coefficient, the spectral 103 radius is numerically computed and discussed. In the section 3, numerical experiments are 104 carried out to show that the conclusions of the eigenvalue analysis hold for multidimensional 105 problems. The conclusions are also verified against a test case of practical interest: the 106 simulation of the natural convection of air due to a large temperature gradient. 107

¹⁰⁹ 2. Analysis of the finite difference preconditioning

110 2.1. HOCS discretization of variable coefficient Poisson's equation

Let us consider the following non-separable Poisson's equation:

$$-\nabla \cdot (\kappa \nabla \phi) = f \tag{1}$$

where κ is a smooth variable coefficient and f the right hand side. Without loose of generality 112 the problem is defined on a cubical domain $\Omega = [0, 1]^3$ for which Neumann or periodic bound-113 ary conditions can be prescribed on the boundary $\Gamma = \partial \Omega$. This equation is the archetype 114 problem occurring in computational fluid dynamics, specifically with incompressible-like 115 models [20, 23] for which the divergence of the velocity have to be exactly enforced. The 116 present analysis focuses on this singular problem which it is known to be among the most 117 tricky part of incompressible-like solvers. So, as commonly encountered with the pressure-118 like variable, the unknown ϕ is cell-centered and the coefficient κ is face-centered. Regardless 119 the discretization, the finite difference approximation of Eq. (1) is formulated in a Cartesian 120 coordinates system as: 121

$$-\left(\delta_x^{fc}\overline{\kappa}^x\delta_x^{cf} + \delta_y^{fc}\overline{\kappa}^y\delta_y^{cf} + \delta_z^{fc}\overline{\kappa}^z\delta_z^{cf}\right)\phi = f \tag{2}$$

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where δ_{ξ} denotes the derivative operator in the ξ -direction, the superscript fc and cf refers to face-to-cell and cell-to-face respectively. The notation $\overline{\kappa}^{\xi}$ refers to the variable coefficient evaluated at the faces in the ξ -direction. Let us define the uniform step size $h_{\xi} = \ell_{\xi}/n_{\xi}$, so the cell and face centres are located at $\xi_i = (i-1/2)h_{\xi}$, $0 \le i \le n_{\xi}+1$ and $\xi_{i+1/2} = i h_{\xi}$, $0 \le i \le n_{\xi}$, respectively.

The discrete approximation of the non-separable Poisson equation Eq. (2) is based on HOCS [13]. According to the mesh staggering, the HOCS derivatives from *cell-to-face* δ_{ξ}^{cf} are given by:

$$\beta\phi_{i-2}' + \alpha\phi_{i-1}' + \phi_i' + \alpha\phi_{i+1}' + \beta\phi_{i+2}' = a\frac{\phi_{i+1/2} - \phi_{i-1/2}}{h_{\xi}} + b\frac{\phi_{i+3/2} - \phi_{i-3/2}}{3h_{\xi}} + c\frac{\phi_{i+5/2} - \phi_{i-5/2}}{5h_{\xi}}$$
(3)

¹³⁰ whereas the *face-to-cell* derivative δ_{ξ}^{cf} is given by the space-shift of the former relation:

$$\beta \phi_{i-3/2}' + \alpha \phi_{i-1/2}' + \phi_{i+1/2}' + \alpha \phi_{i+3/2}' + \beta \phi_{i+5/2}' = a \frac{\phi_{i+1} - \phi_i}{h_{\xi}} + b \frac{\phi_{i+2} - \phi_{i-1}}{3h_{\xi}} + c \frac{\phi_{i+3} - \phi_{i-2}}{5h_{\xi}}$$
(4)

The coefficients α , β , a, b and c are computed to ensure the constraints on the accuracy [13]. The HOCS discretizations used in this work are tabulated in the Tab. 1.

For the periodic boundary conditions, these relations uniquely define the discretization of the Poisson's equation Eq. (1). For the Neumann boundary conditions, lower-order upwind boundary relations are derived [13]. For instance, the following third-order boundary conditions are considered [19]:

$$\phi_{1/2}' + 23\phi_{3/2}' = -25\phi_0 + 26\phi_1 - \phi_2 \tag{5}$$

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$$\phi_{1/2}' - \phi_{3/2}' = -\phi_0 + 2\phi_1 - \phi_2 \tag{6}$$

Because of the implicit formulation of the compact schemes and the staggered grid, the linear system arising from the HOCS discretization of Eq. (2) is no longer sparse. Solutions can be computed by the successive diagonalization solver [10, 19, 27]. The non-separable feature of the Poisson's equation Eq. (1) precludes this direct solver, and iterative ones remain a
natural way to consider. The present study focuses on the second-order finite differences
preconditioning of the non-separable Poisson's equation discretized with HOCS. According
to Haldenwang et al. [10], an eigenvalue analysis of the preconditioned Richardson iterations
method is investigated in the following.

147

148 2.2. Preconditioned Richardson iterations

The analysis of the second-order finite difference preconditioning for the HOCS discretization of the Poisson equation relies on an eigenvalue analysis of the iteration matrix of the Richardson method. This is motivated by the existence of several results for the convergence rate estimates [10, 26]. The preconditioned Richardson iteration is defined by the sequence:

$$\phi^{(k+1)} = \phi^{(k)} - \omega H^{-1} r^{(k)}, \quad 0 \ge k \tag{7}$$

where ω is a relaxation factor, $r^k = L\phi^{(k)} - f$ denotes the residual at the iteration k and L stands for an HOCS discretization of Eq. (2). The notation H^{-1} refers to the preconditioning method which is designed to ensure a good convergence of the sequence Eq. (7), and also to be easily computed. Hence, a classical result is the derivation of the optimal relaxation factor ω_{opt} and convergence rate r_{opt} :

$$\omega_{opt} = 2/(\lambda_{max} + \lambda_{min}) \quad r_{opt} = (\lambda_{max} - \lambda_{min})/(\lambda_{max} + \lambda_{min}) \tag{8}$$

where λ_{min} and λ_{max} stand for the lowest and largest eigenvalues of the preconditioned problem $H^{-1}L$.

For the Poisson equation with a constant coefficient κ defined on a one-dimensional periodic domain, a theoretical framework exists to derive the convergence rate from the preconditioned Richardson method. Indeed, the eigenvectors of the second-order and the HOCS finite differences Eq. (2) are similar. The eigenvectors are expressed as $v_k = \exp(ik2\pi/n), 1 \le k \le$ n, and therefore the eigenvalues are derived from the Fourier analysis of the finite difference schemes. H and L being respectively associated to the second-order finite difference and the HOCS discretization of the one-dimensional version of Eq. (2), the discrete eigenvalues are given by [13]:

$$\lambda_k(H) = \frac{\sin^2(w_k/2)}{4h^2},$$
(9)

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1

$$\lambda_k(L) = \frac{1}{4h^2} \left(\frac{a\sin(w_k/2) + b/3\sin(3w_k/2) + c/5\sin(5w_k/2)}{1 + 2\alpha\cos(w_k) + 2\beta\cos(2w_k)} \right)^2 \tag{10}$$

with $w_k = 2k\pi/n$. Since H and L share the same eigenvectors, the eigenvalues of the preconditioned Poisson problem are determined by $\lambda_k(H^{-1}L) = \lambda_k(L)/\lambda_k(H)$. The Fig. 1 presents the eigenvalues $\lambda_k(H^{-1}L)$ with respect to the HOCS listed in Tab. 1.

The curves in Fig. 1 show that the set of eigenvalues remains bounded by the values at the limit of vanishing w = 0 and at $w = \pi$:

$$\lambda_{min} = \left(\frac{a+b+c}{1+2\alpha+2\beta}\right)^2, \quad \lambda_{max} = \left(\frac{a+b/3+c/5}{1+2\alpha+2\beta}\right)^2 \tag{11}$$

It should be noted that $\lambda_{min} = 1$ because the accuracy requirement in the derivation of the compact scheme needs to satisfy to $1 + 2\alpha + 2\beta = a + b + c$ [13]. Thus, the condition number of the preconditioned iteration matrix is determined by the maximal eigenvalue λ_{max} . In this specific case, the estimation of the preconditioned Richardson's convergence rate is clearedup. Tab. (2) details the spectral radius, and the underlying optimal relaxation factor and the convergence rate for the six schemes. (2).

The eigenvalues of the preconditioned operator $H^{-1}L$ are not dependent on the space size *h*. This result means that if the preconditioner H^{-1} scales like a multigrid method then the higher-order accuracy is achieved with a linear complexity algorithmic because the HOCS residual is itself computed with a linear algorithm complexity. The best convergence rate holds for the fourth-order compact scheme $H_4 tri$, the worst holds for H10pen. The following

conclusion can be drawn: the more accurate is the scheme, the worse is the convergence. 187 Thus, with the scheme H10pen, the convergence rate falls down to 0.29 which is less than 188 two times more than the scheme H4tri. As indicated in the textbook of Canuto et al. [5] and 189 observed by Abide et al. [28], the present analysis remains valid for multidimensional Pois-190 son's equation. In the case of general Poisson equation, which involves a variable coefficient 191 for instance, there is no exact derivation of the eigenvalues. Nevertheless, the eigenvalues of 192 the preconditioned operator can be computed numerically. In the following, this procedure 193 is considered as an alternative to the exact derivation. 194

The brute-force approach consists in assembling the matrices arising from the secondorder and the HOCS discretizations H and L, and then to compute the eigenvalues. Clearly, this procedure depends on the mesh size N, excepted for the periodic case and the constant coefficient for which this approach is exact. For the other cases, a second-order convergence of the numerical error with respect to the mesh size N of the couple of eigenvalues $(\lambda_{min}, \lambda_{max})$ is observed (Fig. 2).

201

[Figure 2 about here.]

It is worth mentioning that the numerical error is computed from the reference eigenvalue computed with the finest mesh N = 256. The Fig. 2 presents the numerical errors in the three schemes H4tri, H6tri and H6pen with Neumann boundary conditions. A -2 slope is noted, thus the Richardson extrapolation is considered to estimate the couple of extreme eigenvalues. The resulting data are presented in Tab. 3.

It should be noted that the results are identical up to two digits. This procedure is considered
hereinafter to assess the preconditioning for the variable coefficient case.

210 2.3. Preconditioning with variable coefficients

The second-order finite differences preconditioning is assessed for a variable coefficient κ and both periodic and Neumann boundary conditions. Specifically, the two following variable ²¹³ coefficients κ in Eq. (1) are considered:

$$\kappa_1(x) = 1 + \frac{9}{10}\sin(4\pi x)$$
(12)

$$\kappa_2(x) = \frac{2}{1 + \epsilon + (1 - \epsilon)\sin(4\pi x)}$$
(13)

where ϵ is a parameter which defines the stiffness of the coefficient ($\epsilon = 10^{-3}$). The coefficients κ_1 , and κ_2 exhibit variations of O(1) and $O(10^3)$ while being continuous. The Richardson extrapolation of the extreme eigenvalues for the preconditioned operator $H^{-1}L$ is detailed in the Tab. 4.

The eigenvalues are close to those derived with the constant coefficient assumption and discussed in the section 2.2. Small discrepancies are observed especially with the stiff coefficient κ_2 . This can be attributed to an under-resolved mesh unable to describe the stiff variations of κ_2 . A similar conclusion to the exact derivation of the convergence rate (Sec. 2.2) can be drawn: the spectral radius does not depend on the mesh size N. In addition no noticeable dependency on the coefficients κ is noted.

A similar analysis is carried out with the Neumann boundary conditions. Thus, the extreme eigenvalues are computed for the schemes H_4tri , H6tri and H6pen. The results are presented in Tab. 5.

228

[Table 5 about here.]

The bounds of the eigenvalues are similar to those derived in the section (2.2) Eq. (11). The slight observed deviations can be explained by a coarse mesh which seems to be insufficient to describe the stiff variations of the coefficients κ .

To summarise the findings, the eigenvalues bound of the preconditioned operator $H^{-1}L$ is not sensitive to the mesh size N [19]. Moreover, a finite difference preconditioning based on a variable coefficient Poisson equation leads also to an eigenvalue bound independent from the variable coefficient. This feature has two main consequences. First, this shows a way to design a HOCS Poisson solver for non-separable problems which could not depend on the
variable coefficient. Secondly, if the preconditioning step is efficiently performed, the method
could benefit from High Performance Computing. It's because the HOCS residual can be also
calculated with a linear algorithmic complexity while involving only halo exchange parallel
communications [19].

241 2.4. Implementation

The preconditionned Richardson sequence Eq. (7) relies on the evaluation of the HOCS 242 residual Eq. (2) and on the solution of the second-order discretization of Eq. (1) H^{-1} . The 243 evaluation of the preconditioning H^{-1} has to be performed efficiently to ensure correct overall 244 performance. A review on the fast Poisson solver is proposed in the reference [4]. According 245 to this review, FFT based solvers are among the most efficient for problems involving a 246 constant coefficient. Otherwise, multigrid methods are shown to be suitable. Although, 247 geometric multigrid methods are usually more efficient than algebraic multigrids for Poisson's 248 equation on cubical domains [4], in this work, the AGMG library developed by Notay [1] 249 is used. This choice is motivated by the user friendly interface, the black-box mode and 250 its parallel implementation. It is worth mentioning that in each Richardson iteration of 251 the sequence Eq. (7) only two or three iterations of the algebraic multigrid are performed. 252 It has been experienced that only an approximate solving H^{-1} is sufficient to achieve the 253 global convergence of the Richardson sequence. The method has been implemented using a 254 previous parallel code dedicated to compact scheme discretizations [19]. 255

256 3. Numerical results

This section is devoted to the assessment of the second-order finite difference preconditioning for a HOCS discretization of the non-seperable Poisson equation. First the effective accuracy of the present solver implementation is demonstrated. Then, the extreme eigenvalues are estimated from numerical experiments including numerical solution of Poisson's equation and the simulation of the unsteady natural convection in a tall cavity. This former numerical experiment aims to illustrate the finite differences preconditioning in a more ²⁶³ general context.

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264 3.1. HOCS accuracy verification

The accuracy of the HOCS discretizations for the problem Eq. (1) is verified. The method consists in computing the numerical error for several grid sizes in order to estimate the effective order of accuracy. A cubical domain is considered $\Omega = [0, 2\pi]^3$, with either periodic boundary or Neumann boundary conditions. The right-hand side of the Poisson equation is derived from the exact solution:

$$\phi = \cos(2\pi x)\cos(2\pi y)\cos(2\pi z) \tag{14}$$

and the following three-dimensional extensions of the coefficients Eq. (12) is considered:

$$\kappa_1 = 1 + \frac{9}{10} \sin(4\pi x) \sin(4\pi y) \sin(4\pi z)$$
(15)

$$\kappa_2 = \frac{2}{1 + \epsilon + (1 - \epsilon)\sin(4\pi x)\sin(4\pi y)\sin(4\pi z)}$$
(16)

The solutions are computed with the preconditioned Richardson sequence Eq. (7). In the case of Neumann boundary conditions the mesh is refined at the boundary according to a tangent hyperbolic mesh transformation [27]. Fig. 3 presents the numerical error with respect to the mesh size N for the coefficient κ_2 .

Fig. 3-a shows that the numerical errors decrease linearly with the expected slopes. It is also noted that the numerical error for the scheme H10pen saturates beyond N = 64 nodes because the machine accuracy is reached. Fig. 3-b corresponds to the Neumann boundary conditions. The slopes also agree with the expected HOCS's accuracy. These numerical experiments confirm that the present implementation of the preconditioned Richardson iterations fulfils the accuracy requirements.

282 3.2. Assessment of the preconditioning

The validity of the spectral radius predictions established in the section 2 is verified from the residual history of the Richardson iterations method. Indeed, the knowledge of the convergence rate r_{opt} and the optimal relaxation factor ω_{opt} allows us to estimate the couple of extreme eigenvalues ($\lambda_{min}, \lambda_{max}$) from the relations Eq. (8). The convergence rate r_{opt} is computed from the residual slope [22]:

$$r = (m_2 - m_1) \sqrt{\frac{r_{m_1}}{r_{m_2}}} \tag{17}$$

where m_1 , m_2 denote two iteration numbers, and r_{m_1} , r_{m_2} the associated residual respectively. The residual history is obtained from the zero solution of Poisson's equation and using a random field as initial guess [22]. Fig. 4 presents the residuals for the scheme *H8tri*, the variable coefficient κ_2 with periodic boundary conditions.

First, it is observed that the convergence rate is slightly dependent on the mesh size N, 293 but the slope reaches a limit as the mesh is refined. From the residual history observed 294 on the finest grid and using the relation Eq. (17), the convergence rate is estimated at 295 $r_{opt} = 0.29$. It is worth mentioning that the relaxation factor of the Richardson sequences 296 Eq. (17) is initialized to the optimal value detailed in Tab. 2. In this case, the estimate of the 297 spectral bound for the preconditioned Richardson iterations is $(\lambda_{min}, \lambda_{max}) = (1.01, 1.82).$ 298 This result agrees with the eigenvalue analysis of the section 2. It should be noted that this 299 result validates the value of the optimal factor ω_{opt} . 300

The sensitivity of the convergence rate evaluation to the mesh size is investigated. Fig. 5 presents the convergence rate r_{opt} with respect to the mesh size for the HOCS discretizations and for the variable coefficient κ_2 .

304

[Figure 5 about here.]

These curves show a small dependency on the convergence rate to the mesh size above grids of size 128³. This result holds for both periodic and Neumann boundary conditions. This confirms the main result of the section 2 which highlights that the convergence rate is not dependent on the mesh size, and thus, even if a stiff variable coefficient is used. In the following the convergence rate will be estimated from the finest grid 256³.

The spectral bounds of the iteration matrix is measured for each HOCS scheme. Tab. 6 and Tab. 7 present the extreme eigenvalues $(\lambda_{min}, \lambda_{max})$ computed from the residual curves on the finest grid 256³. First, for experiments involving periodic boundary conditions (Tab. 6), one can observed that for each discretization the couple of extreme eigenvalues are close to those predicted in the section 2.

Thus, the minimal eigenvalue λ_{min} ranges between 1.00 and 1.02 while the expected value is 316 1. Next, it is observed that the maximal eigenvalue λ_{max} is also close to the one predicted 317 by the one-dimensional analysis developed in the section 2 (Tab. 2). This holds for the 318 constant and both variable coefficients κ_1 and κ_2 . These numerical experiments corroborate 319 the conclusion drawn in the section 2 on the properties of the second-order preconditioning: 320 the independence of the convergence rate with respect to the mesh size and the coefficient 321 κ . The table 7 presents the two extreme eigenvalues in the case of prescribed Neumann 322 boundary conditions. 323

The computed eigenvalues are also similar to the prediction of the Tab. 2. This shows that despite the Neumann boundary conditions the eigenvalues spectra remains bounded.

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To illustrate the implications of this preconditioning on the wall time, the former is reported for several mesh sizes in table 8. Thus, the wall time is defined as the time necessary to decrease the residual to 10^{-9} in case of a periodic domain, for the coefficient κ_2 and with the scheme *H6tri*. In addition, the wall time of the multigrid AGMG preconditioner, and the wall time of the Conjugated Gradient to get the same level of residual are also reported.

[Table 8 about here.]

First, one can note that the wall time of the multigrid preconditioning is almost the wall 335 time of the preconditioned Richardson. This means that a higher accuracy is obtained at the 336 cost of a second order discretization solved by a multigrid method. Since multigrid meth-337 ods are known to scale linearly with the number of unknowns, it is expected that compact 338 scheme discretizations of elliptic problems inherit of this scaling. Then, it is observed that 339 the Conjugated Gradient perform well than preconditioned Richardson for coarser meshes 340 than 32^3 . In other hand for finer meshes than 32^3 , it is the preconditioned Richardson which 341 performs well. Indeed, in the absence of a preconditioning the number of iterations increases 342 significantly with the problem size and the underlying ill-conditioning. 343

The present test confirms that the preconditioning is not sensitive to the Neumann/periodic boundary, to the mesh size and to the coefficient κ , at least for continuous one. However, these conclusions concern the model coefficients κ_1 and κ_2 . To extend the conclusions to more general coefficients, the simulation of a variable density flow is considered in the following.

348 3.3. Unsteady natural convection in a tall cavity

Let us consider the flow in a closed cavity with large temperature gradients. The low Mach number formulation of the Navier-Stokes equations may be considered as an alternative to the Boussinesq approximation for accounting buoyancy forces and density variations. A common way to address the simulations of such flow consists in solving a non-separable Poisson equation to enforce the final divergence of the velocity [20, 23]. This equation reads:

$$\nabla \cdot \frac{1}{\rho} \nabla \Phi = \nabla \cdot (\mathbf{u}^* - S) \tag{18}$$

where Φ denotes the pressure-like variable, \mathbf{u}^* the provisional velocity, ρ the variable density and S the divergence to enforce. Knikker [20] proposed a detailed review of these approaches. In what follows, the denoted P1-A1 in [20] has been implemented with an in-house code devoted to the simulation of turbulent flows [28–30]. The velocity, pressure and temperature are located on a staggered grid, the time advancement is based on the semi-implicit Adams Bashforth/Runge Kutta scheme and HOCS *H4tri*, *H6tri* and *H6pen* are considered. First,
the space accuracy of the present low Mach solver is demonstrated using the Method of
Manufactured Solutions [31]. According to the validation procedure of Bouloumou et al.
[32], the following two-dimensional analytical solution is considered:

$$u(x, y) = +\cos x \sin y + \frac{1}{\Pr\sqrt{\text{Ra}}} \cos x \sin y$$

$$v(x, y) = -\sin x \cos y + \frac{1}{\Pr\sqrt{\text{Ra}}} \sin x \cos y$$

$$p(x, y) = \cos x \cos y$$

$$T(x, y) = 1 + \epsilon \sin x \sin y$$

$$\rho(x, y) = P_{th}/T(x, y)$$

$$P_{th} = 1$$

(19)

with $Ra = 10^3$, Pr = 0.71 and $\epsilon = 0.5$. Both periodic and Dirichlet boundary conditions 363 (non-periodic) in a square computational domain $\Omega = [0, 2\pi] \times [0, 2\pi]$ are considered. It 364 is worth mentioning that the analytical solution is a the non-solenoidal velocity field which 365 is specific to the low Mach model. The numerical error is computed with the L2-norm of 366 the difference between the exact and the numerical solution. The numerical error of the 367 pressure p is reported in the figure 6 for each discretization H4, H6tri and H6pen. For the 368 sake of clarity, the analysis based on the velocity and on the temperature are not reported 369 because of the numerical error slopes are similar to the pressure one. 370

[Figure 6 about here.]

371

The slopes of the numerical error show the fourth and the sixth-order accuracy of the implemented code for periodic boundary conditions (Fig. 6). The same conclusion holds for the non-periodic conditions with a slightly above slope that the expected one. For instance, the slopes of 5.7 and 5.6 are noted for the tridiagonal and pentadiagonal sixth-order compact schemes.

³⁷⁷ In addition, the present low Mach solver is validated against the steady natural convection

flow in a differentially heated cavity with a large temperature gradient. The configuration 378 flow is detailed in the Benchmark [6]. The control flow parameters are the Rayleigh num-379 ber, the deviation to the Boussinesq approximation set to $\epsilon = 0.6$ and the Prandlt number 380 Pr = 0.71. The thermophysical properties are constant. A grid sensitivity analysis is 381 performed to assess the accuracy of the present low Mach solver at the Rayleigh number 382 $Ra = 10^5$. First, a fine grid solution has been computed on a mesh of size 120×120 and 383 with the small CFL number 0.05. This simulation leads to a Nusselt number Nu = 4.5516384 and a thermodynamic pressure $P_{th}/P_0 = 0.8518$, which agrees the values computed in [32] 385 and [33]. Fig. 7 presents, for the grid sizes N = 32, 48 and 64, the absolute difference with 386 the fine grid solution of the Nusselt number and thermodynamic pressure. 387

[Figure 7 about here.]

The slopes confirm the expected accuracy, and even show a saturation due to the low level error for the two sixth-order schemes. A further validation is performed with a higher Rayleigh number $Ra = 10^6$. For a mesh of size 128×128 , the computed Nusselt number is Nu = 8.8598 and the final thermodynamic pressure $P_{th}/P_0 = 0.856338$, which agree well with the reference solution [6]. Fig. 8 presents the streamlines and the isolines of the temperature.

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[Figure 8 about here.]

Both plots are in agreement with the results of Heuveline [34]. The present low Mach solver implementation being validated, one can focus on the spectrum of the finite difference preconditioning.

To this end, the unsteady natural convection in a tall cavity is considered [35, 36]. The aspect ratio of the cavity is 1:8, the Rayleigh number is $Ra = 10^6$ and the normalized temperature difference is $\epsilon = 0.8$. This former parameter is sufficiently high to lead to a strongly unsteady flow with large density variations: the order of magnitude is one. The simulations of the flow are carried out up to a dimensionless time t = 1000 with a CFL number of 0.8 and using a fine mesh 128×512 . Fig. 9 presents a temporal snapshot sequence of the isolines of temperature. The contours plots agree qualitatively with those recently published [35, 36]. The convergence rate of the Richardson iterations sequence is measured for the three discretizations H4tri, H6tri and H6pen using the procedure detailed in the section 3.2. Thus, the maximum of the residual Eq. (7) with respect to the Richardson iteration number *it* is plotted in Fig. 10 for one temporal iteration of the Navier-Stokes solver. It should be mentioned that the iterative procedure Eq. (7) has been initialized with $\phi = 0$ and was stopped when the residual is below $||r|| < 10^{-10}$.

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420

[Figure 10 about here.]

Also, it has been observed that whatever the time step the slopes of Fig. (8), the curves remain of similar slope. This observation confirms that a such low-order preconditioning is not sensitive to the variable coefficient ρ . For this mesh size, the solution of time of the pressure equation is about 1.1 s with 24 processors. The measured convergence rates on Fig. (8) and the associated extrem eigenvalues are summarized in Tab. 9.

The assessed extrem eigenvalues agree the theoretical estimates of the section 2. It should be noticed that the spectrum of the preconditioned operator is slightly smaller. This can be explained by the cancellation of the high-frequency fluctuations due to the fine mesh or the compact schemes cut-off [13]. This test confirms that the second-order finite difference preconditioning of HOCS compact schemes for non-separable Poisson's equation possess a bounded spectrum independent to the variable coefficient.

427 4. Conclusion

An analysis of the second-order finite-difference preconditioning of the higher-order compact scheme discretization regarding the variable coefficient Poisson equation is presented in this work. In particular, it is demonstrated that the preconditioner built from the second-order finite-difference discretization leads to an iterative Richardson method that the
convergence rate is not sensitive to the mesh size and the variable coefficient. The finding
is even more valuable that this preconditioning can be applied on the conservative form of
the Poisson's equation, the one involved in some discretizations of variable density flows for
instance.

Several numerical experiments based on manufactured solutions demonstrate the accu-436 racy of the discretization up to the tenth-order. The convergence rate of the present lower-437 order preconditioned Richardson method has been found not sensitive to the mesh-size and 438 the variable coefficient. This former finding is verified with a more general variable-coefficient 439 test case: variable density flow occurring in a strongly heated cavity. This demonstrates the 440 relevance of the lower-order preconditioning for the compact scheme discretizations even the 441 more that the present solver involves numerical methods with linear computational complex-442 ity. 443

Further investigations would to put forward a such low-order preconditioning as a simple way to achieve simultaneously scalable algorithm and higher-order accuracy, and thus to take full advantage of the High Performance Computing.

447

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540 List of Figures

541	1	Eigenvalues of the preconditioned problem $H^{-1}L$ for several HOCS discretiza-	
542		tions	25
543	2	Mesh convergence of the spectral radius of $H^{-1}L$: Neumann boundary condi-	
544		tions and constant coefficient.	26
545	3	Assessment of the order of accuracy: variable coefficient κ_2	27
546	4	Mesh sensitivity of the residual history: periodic domain and coefficient κ_2 .	28
547	5	Mesh sensitivity of the convergence rate: periodic domain and coefficient κ_2 .	29
548	6	The numerical errors of the pressure variable.	30
549	7	Grid sensitivity analysis of the differentially heated cavity at $Ra = 10^5$	31
550	8	Natural convection in a square cavity: $(Ra, \epsilon, Pr) = (10^6, 0.6, 0.71)$ and con-	
551		stant properties.	32
552	9	Snapshots of 15 isolines of temperature ranging in 0.3 and 1.7: $(Ra, \epsilon, Pr) =$	
553		$(10^6, 0.8, 0.71)$	33
554	10	Natural convection in the tall cavity: residual history of the preconditioned	
555		Richardson iteration.	34



Figure 1: Eigenvalues of the preconditioned problem $H^{-1}L$ for several HOCS discretizations.



Figure 2: Mesh convergence of the spectral radius of $H^{-1}L$: Neumann boundary conditions and constant coefficient.



Figure 3: Assessment of the order of accuracy: variable coefficient κ_2 .



Figure 4: Mesh sensitivity of the residual history: periodic domain and coefficient κ_2 .



Figure 5: Mesh sensitivity of the convergence rate: periodic domain and coefficient κ_2 .



Figure 6: The numerical errors of the pressure variable.



Figure 7: Grid sensitivity analysis of the differentially heated cavity at $Ra = 10^5$.



(a) Isolines of temperature



Figure 8: Natural convection in a square cavity: $(Ra, \epsilon, Pr) = (10^6, 0.6, 0.71)$ and constant properties.



Figure 9: Snapshots of 15 isolines of temperature ranging in 0.3 and 1.7: $(Ra, \epsilon, Pr) = (10^6, 0.8, 0.71)$.

Figure 10: Natural convection in the tall cavity: residual history of the preconditioned Richardson iteration.

556 List of Tables

557	1	Compact scheme coefficients for the first derivative defined on a staggered grid.	36
558	2	The lowest and largest eigenvalues of the preconditioned operator $H^{-1}L$ and	
559		the underlying optimal parameters for the preconditioned Richarson iterations.	37
560	3	The lowest and largest eigenvalues of the preconditioned Richardson method:	
561		Neumann boundary conditions and constant coefficient.	38
562	4	The lowest and largest eigenvalues of the preconditioned Richardson method:	
563		periodic boundary conditions and variable coefficient	39
564	5	The lowest and largest eigenvalues of the preconditioned Richardson method:	
565		Neumann boundary conditions and variable coefficient	40
566	6	Estimates of the lowest and largest eigenvalues of the preconditioned Richard-	
567		son method: periodic boundary conditions and variable coefficient	41
568	7	Lowest and largest eigenvalues estimates of the preconditioning : Neumann	
569		boundary conditions and variable coefficient	42
570	8	Wall time in second to solve the Poisson equation with the variable coefficient	
571		κ_2 . Notations: Conjugate Gradient (CG), Richardson preconditioned (PR)	
572		by the algebraic multigrid AGMG.	43
573	9	Estimates of the textcolorblueextrem eigenvalues evaluated from the simula-	
574		tion of the tall cavity flow	44

name	order	α	β	a	b	С
H4tri	h^4	1/22	0	12/11	0	0
H6tri	h^6	9/62	0	63/62	17/62	0
H6pen	h^6	154/1289	-17/5178	960/863	0	0
H8tri	h^8	25/118	0	2675/2832	925/1888	-61/5664
H8pen	h^8	6114/25669	183/51338	23400/25669	14680/25669	0
H10pen	h^{10}	96850/288529	9675/577058	683425/865587	505175/577058	69049/1731174

Table 1: Compact scheme coefficients for the first derivative defined on a staggered grid.

scheme	H4tri	H6tri	H6pen	H8tri	H8pen	H10pen
λ_{min}	1.00	1.00	1.00	1.00	1.00	1.00
λ_{max}	1.44	1.70	1.62	1.83	1.84	1.95
$r_{\rm opt}$	0.18	0.26	0.24	0.29	0.30	0.32
$\omega_{ m opt}$	0.82	0.74	0.76	0.71	0.70	0.68

Table 2: The lowest and largest eigenvalues of the preconditioned operator $H^{-1}L$ and the underlying optimal parameters for the preconditioned Richarson iterations.

scheme	H4tri	H6tri	H6pen
λ_{min}	1.00	1.00	1.00
λ_{max}	1.44	1.70	1.62

Table 3: The lowest and largest eigenvalues of the preconditioned Richardson method: Neumann boundary conditions and constant coefficient.

case	scheme	H4tri	H6tri	H6pen	H8tri	H8pen	H10pen
κ_2	λ_{min}	1.00	1.00	1.00	1.00	1.00	1.00
κ_2	λ_{max}	1.44	1.70	1.62	1.83	1.85	1.95
κ_3	λ_{min}	0.99	0.99	0.99	0.99	0.99	0.99
κ_3	λ_{max}	1.45	1.70	1.62	1.83	1.85	1.95

Table 4: The lowest and largest eigenvalues of the preconditioned Richardson method: periodic boundary conditions and variable coefficient.

case	scheme	H4tri	H6tri	H6pen
K	λ_{min}	1.00	0.98	1.00
κ_1	λ_{max}	1.44	1.70	1.62
10	λ_{min}	1.00	0.99	0.99
<i>κ</i> ₂	λ_{max}	1.45	1.72	1.64

Table 5: The lowest and largest eigenvalues of the preconditioned Richardson method: Neumann boundary conditions and variable coefficient.

case	scheme	H4tri	H6tri	H6pen	H8tri	H8pen	H10pen
constant	λ_{min}	1.01	1.02	1.02	1.02	1.02	1.02
constant	λ_{max}	1.43	1.68	1.60	1.81	1.82	1.93
10	λ_{min}	1.00	1.02	1.01	1.01	1.02	1.02
κ_1	λ_{max}	1.44	1.68	1.61	1.81	1.82	1.93
10	λ_{min}	1.01	1.01	1.01	1.01	1.01	1.01
κ_2	λ_{max}	1.43	1.69	1.61	1.82	1.84	1.94

Table 6: Estimates of the lowest and largest eigenvalues of the preconditioned Richardson method: periodic boundary conditions and variable coefficient.

case	scheme	H4tri	H6tri	H6pen
constant	λ_{min}	1.01	1.01	1.02
constant	λ_{max}	1.43	1.68	1.60
16	λ_{min}	1.01	1.02	1.01
κ_1	λ_{max}	1.43	1.68	1.61
K	λ_{min}	0.98	1.01	0.99
n2	λ_{max}	1.46	1.69	1.63

Table 7: Lowest and largest eigenvalues estimates of the preconditioning : Neumann boundary conditions and variable coefficient.

N	CG	AGMG	\mathbf{PR}
16^{3}	0.02	0.43	0.47
32^{3}	0.42	1.69	1.96
48^{3}	4.64	3.54	3.80
64^{3}	17.42	8.33	8.99
96^{3}	247.80	23.00	25.61

Table 8: Wall time in second to solve the Poisson equation with the variable coefficient κ_2 . Notations: Conjugate Gradient (CG), Richardson preconditioned (PR) by the algebraic multigrid AGMG.

scheme	H4tri	H6tri	H6pen
r	0.17	0.24	0.23
λ_{min}	1.01	1.02	1.01
λ_{max}	1.43	1.68	1.61

Table 9: Estimates of the text colorblueextrem eigenvalues evaluated from the simulation of the tall cavity flow.