Compact finite difference schemes of arbitrary order for the Poisson equation in arbitrary dimensions

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Abstract A formulation of the Taylor expansion with symmetric polynomial algebra allows to compute the coefficients of compact finite difference schemes, which solve the Poisson equation at an arbitrary order of accuracy on a uniform Cartesian grid in arbitrary dimensions. This construction produces original high order schemes which respect the *Discrete Maximum Principle*: a tenth order scheme in dimension three and several sixth order schemes in arbitrary dimension. Numerical experiments validate the accuracy of these schemes.

Keywords High order compact solver · finite difference schemes · Poisson equation · symmetric polynomials

Mathematics Subject Classification (2000) MSC 65N02 · MSC 65Y02

Introduction

In his book *Numerische Behandlung von Differentialgleichungen* written in 1951 and translated into English in 1966 with the title *The numerical treatment of differential equations* [3], Lothar Collatz introduced the idea of disturbing the right-hand member of the Poisson equation:

$$\Delta u = v \quad \text{with} \quad \Delta u = \sum_{i=1}^{d} \partial_i^2 u \tag{0.1}$$

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to increase the accuracy of the finite difference schemes on Cartesian grids with a mesh $h > 0$, without increasing the size of the associated stencil $(\alpha_{\boldsymbol{\ell}})$:

$$\frac{1}{h^2} \sum_{\boldsymbol{\ell} \in \mathbb{Z}^d} \alpha_{\boldsymbol{\ell}}\, u(\mathbf{x}_h + \boldsymbol{\ell} h) = \sum_{\boldsymbol{\ell} \in \mathbb{Z}^d} \beta_{\boldsymbol{\ell}}\, v(\mathbf{x}_h + \boldsymbol{\ell} h), \quad \forall \mathbf{x}_h \in \mathring{\Omega}_h. \tag{0.2}$$

This kind of schemes is coined the "Mehrstellenverfahren" or Hermitian formulas, or more simply *compact* finite difference scheme.

As explained in [3] the coefficients $(\alpha_{\boldsymbol{\ell}})$ and $(\beta_{\boldsymbol{\ell}})$ are derived from the Taylor formulae applied to $u(\mathbf{x} + \boldsymbol{\ell} h)$ and $v(\mathbf{x} + \boldsymbol{\ell} h)$ (with v supposedly equal to Δu) by canceling the terms up to the highest order in h as possible. He extended this principle to other operators and other grids than the Cartesian one. In an appendix, he made a list of two-dimensional schemes from [1] or that he had obtained, with their precise accuracy errors.

The extension to the three-dimensional case is known as the *HOC Stencil*, standing for "High Order Compact Stencil". This was introduced in [1,19] and tested in [21]. It allows the Poisson equation to be solved at the sixth order of accuracy; for a smooth function the error behaves as $O(h^6)$.

This type of scheme is classical in Numerical Analysis manuals. The interests of compact stencils compared to simple ones are discussed in reference articles such as [13] or reference textbooks such as [11]. This latter proposes a very interesting fourth order compact scheme in an arbitrary dimension as an exercise. It also states that "it might require manipulation and unwieldy algebra" to generalize the "Mehrstellenverfahren" schemes, without indicating how to go further. In [17] the author considers the case of grids with different mesh sizes depending on the direction. It generalizes finite difference compact schemes to arbitrary dimensions while they remain accurate to the fourth order.

Compared to the explicit Laplace discrete formulas, the valuable properties of these numerical schemes are: the order of accuracy, the compactness, the robustness in iterative algorithms and the spectral accuracy. The diameter of the stencil is critical in adaptive grids where we do not want to fetch distant points.

But the most important property of the compact schemes, which greatly impact their stability, is the ability of some of them to conserve the *Maximum Principle* [14]: $\alpha_{\mathbf{0}} < 0$ and $\alpha_{\boldsymbol{\ell}} \geq 0$ for $\boldsymbol{\ell} \neq \mathbf{0}$ in (0.2). Untill recently there was no available compact scheme with this property with a better order than sixth in dimensions two and three, and fourth order in dimensions larger than four. Thanks to the simplification implied by the symmetric polynomials formulation, in the following manuscript we establish such a tenth order scheme in dimension three and such sixth order schemes in arbitrary dimension. These latter schemes are derived once and can be used for any choice of dimension. And it seems that nothing impedes higher orders for the construction of such compact schemes.

This research is motivated by applications such as *ab initio* chemistry [5] which requires a very high accuracy on smooth solutions of the Poisson equation. With Fast Multipole Method [6], finite difference compact schemes associated to multigrid algorithms rank among the best solvers for elliptical equations [18,7,11,23,21]. In a very near future we will extend the adaptive mesh refinement (AMR) fourth-order

two-dimensional Poisson solver presented in [4] to higher order and higher dimensions using the construction presented in this manuscript. These will make *ab initio* chemistry computations possible on unbounded domains thanks to the zooming property of the AMR.

As we will see here and in the AMR forthcoming manuscript, switching the order of accuracy from sixth to tenth allows a gain of few orders of magnitude in the accuracy. This justifies the theoretical developments here in.

Some attempts were made to automate the computation of the coefficients of compact Poisson solvers with naive approaches [9]. But they remained unsuccessful because the number of equations and coefficients makes the task tedious. In particular, it is difficult to see which coefficients should be activated in the sense possibly non zero. In the following manuscript a large part of the complexity disappears thanks to the symmetric Taylor expansion associated with the symmetric stencils that we consider. Based on these considerations, we wrote a small *Scilab* script of approximately 120 lines to compute the systems of equations and the coefficients associated to any symmetric stencils. This script is available on demand to the author. One can pass the linear systems to *Maple* to find the coefficients under their rational forms as they are presented in the manuscript.

In the first part of this manuscript we introduce the notations on symmetric stencils and symmetric polynomials and detail the general construction of the compact schemes for the Poisson equation. In the second part, we compute the coefficients for some specific cases taken from the literature or not. And we list some important properties the schemes should satisfy. Some of the resulting schemes are original and much more accurate than the existing ones. In a third part, we numerically test these compact schemes with the help of multigrid algorithms and prove that they are as accurate as asserted.

1 Notations and preliminary results

1.1 Stencils in multidimensional grids

Since they give a good visualization of the stencil, we use the notations presented in [3,11] for a multi-diagonal linear operator in a Cartesian grid. For instance the original fourth order "Mehrstellenverfahren" scheme in two dimensions appears as:

$$\frac{1}{6h^2}\begin{array}{ccc} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{array} u = \frac{1}{12}\begin{array}{ccc} & 1 & \\ 1 & 8 & 1 \\ & 1 & \end{array} v \tag{1.1}$$

and stands for:

$$\begin{aligned}\frac{1}{6h^2}\,(&-20\,u_{i_1,i_2}+4\,u_{i_1+1,i_2}+4\,u_{i_1-1,i_2}+4\,u_{i_1,i_2+1}+4\,u_{i_1,i_2-1}\\&+u_{i_1+1,i_2+1}+u_{i_1-1,i_2+1}+u_{i_1+1,i_2-1}+u_{i_1-1,i_2-1})\\=\frac{1}{12}\,(&8\,v_{i_1,i_2}+v_{i_1+1,i_2}+v_{i_1-1,i_2}+v_{i_1,i_2+1}+v_{i_1,i_2-1})\end{aligned}$$

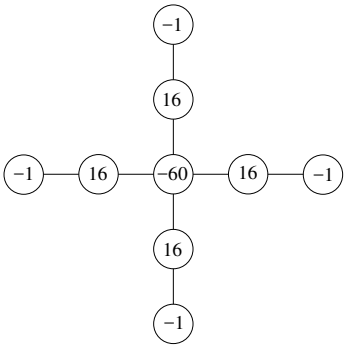
for all couples of integers (i_1,i_2) for which the terms $v_{i_1,i_2}=v(i_1h,i_2h)$, $v_{i_1\pm1,i_2}=v(i_1h\pm h,i_2h)$ and $v_{i_1,i_2\pm1}=v(i_1h,i_2h\pm h)$ are defined and $u_{i_1,i_2}=u(i_1h,i_2h)$ that is to be determined.

For solving the Poisson equation, scheme (1.1) performs much better than the non compact scheme which results from the cumulation of the fourth order one dimensional scheme

$$\frac{1}{h^2}\left[-\frac{1}{12},\frac{4}{3},-\frac{5}{2},\frac{4}{3},-\frac{1}{12}\right]\,u=\partial_x^2u+O(h^4)$$

in the directions x and y. The stencil of the latter is:

$$\frac{1}{12h^2}$$



$$u=v. \tag{1.2}$$

This latter scheme does not satisfy the maximum principle property: $\alpha_{[2\ 0]}<0$. It does not provide good spectral approximation [13] and it poorly preserves the spatial isotropy in wave propagation problems [2].

In the manuscript, we denote A and B the operators attached to (α_ℓ) and (β_ℓ):

$$Au(\mathbf{x})=\sum_{\boldsymbol{\ell}\in\mathbb{Z}^d}\alpha_{\boldsymbol{\ell}}\,u(\mathbf{x}+\boldsymbol{\ell}h)\quad\text{and}\quad Bv(\mathbf{x})=\sum_{\boldsymbol{\ell}\in\mathbb{Z}^d}\beta_{\boldsymbol{\ell}}\,v(\mathbf{x}+\boldsymbol{\ell}h).$$

1.2 Construction by tensorization of the one-dimensional case

Some authors, including [10], have constructed compact finite difference Poisson solvers using tensorization of one dimensional second differentiations. Let p, L_a and L_b be integers such that we have the following compact scheme for the second differentiation:

$$\text{(E)}\quad\frac{1}{h^2}\sum_{\ell=-L_a}^{L_a}a_\ell u_\ell=\sum_{\ell=-L_b}^{L_b}b_\ell\partial^2u_\ell+O\left(h^{2p}\right).$$

Then we have

$$(\mathrm{E}_1) \quad \frac{1}{h^2}\sum_{\ell_1=-L_a}^{L_a} a_{\ell_1} u_{\ell_1\ell_2} = \sum_{\ell_1=-L_b}^{L_b} b_{\ell_1}\partial_x^2 u_{\ell_1\ell_2} + O\left(h^{2p}\right), \quad \forall \ell_2 \in \mathbb{Z},$$

and

$$(\mathrm{E}_2) \quad \frac{1}{h^2}\sum_{\ell_2=-L_a}^{L_a} a_{\ell_2} u_{\ell_1\ell_2} = \sum_{\ell_2=-L_b}^{L_b} b_{\ell_2}\partial_y^2 u_{\ell_1\ell_2} + O\left(h^{2p}\right), \quad \forall \ell_1 \in \mathbb{Z}.$$

Taking

$$\sum_{\ell_2=-L_b}^{L_b} b_{\ell_2} (\mathrm{E}_1)_{\ell_2} + \sum_{\ell_1=-L_b}^{L_b} b_{\ell_1} (\mathrm{E}_2)_{\ell_1},$$

we obtain:

$$\frac{1}{h^2}\left(\sum_{\ell_2=-L_b}^{L_b}\sum_{\ell_1=-L_a}^{L_a} b_{\ell_2} a_{\ell_1} u_{\ell_1\ell_2} + \sum_{\ell_1=-L_b}^{L_b}\sum_{\ell_2=-L_a}^{L_a} b_{\ell_1} a_{\ell_2} u_{\ell_1\ell_2}\right)$$

$$= \sum_{\ell_2=-L_b}^{L_b}\sum_{\ell_1=-L_b}^{L_b} b_{\ell_2} b_{\ell_1}\partial_x^2 u_{\ell_1\ell_2} + \sum_{\ell_1=-L_b}^{L_b}\sum_{\ell_2=-L_b}^{L_b} b_{\ell_1} b_{\ell_2}\partial_y^2 u_{\ell_1\ell_2} + O\left(h^{2p}\right)$$

$$= \sum_{\ell_1=-L_b}^{L_b}\sum_{\ell_2=-L_b}^{L_b} b_{\ell_1} b_{\ell_2}\Delta u_{\ell_1\ell_2} + O\left(h^{2p}\right).$$

We can vary this construction. The stencils in the x and y directions do not have to be the same. The authors of [10] exploit an even different construction which allows them to construct compact finite differences on irregular stencils for immersed boundaries.

In dimension two, let us assume we have a given stencil $B = (\beta_{\ell_1\ell_2})$. In [10] it is derived from the usual stencil B of the tensorized fourth order compact finite difference in the regular case. But it can be any stencil B. Then, following these authors, we construct the fourth order one dimensional compact schemes $(a^1_{\ell_2\ell_1}, \beta_{\ell_1\ell_2})_{\ell_1}$ for all ℓ_2, and $(a^2_{\ell_1\ell_2}, \beta_{\ell_1\ell_2})_{\ell_2}$ for all ℓ_1:

$$\left(\mathrm{E}^1_{\ell_2}\right) \quad \frac{1}{h^2}\sum_{\ell_1} a^1_{\ell_2\ell_1} u_{\ell_1\ell_2} = \sum_{\ell_1} \beta_{\ell_1\ell_2}\partial_x^2 u_{\ell_1\ell_2} + O\left(h^4\right), \quad \forall \ell_2,$$

$$\left(\mathrm{E}^2_{\ell_1}\right) \quad \frac{1}{h^2}\sum_{\ell_2} a^2_{\ell_1\ell_2} u_{\ell_1\ell_2} = \sum_{\ell_2} \beta_{\ell_1\ell_2}\partial_y^2 u_{\ell_1\ell_2} + O\left(h^4\right), \quad \forall \ell_1.$$

Then making

$$\sum_{\ell_2}\left(\mathrm{E}^1_{\ell_2}\right) + \sum_{\ell_1}\left(\mathrm{E}^2_{\ell_1}\right),$$

we obtain:

$$\frac{1}{h^2}\left(\sum_{\ell_1}\sum_{\ell_2}\left(a^1_{\ell_2\ell_1} + a^2_{\ell_1\ell_2}\right) u_{\ell_1\ell_2}\right) = \sum_{\ell_1}\sum_{\ell_2}\beta_{\ell_1\ell_2}\Delta u_{\ell_1\ell_2} + O\left(h^4\right).$$

All the symmetric stencils obtained by this method can be derived by the construction proposed in the present manuscript. And the most interesting cases, in high dimensions or for high orders, can not be derived by the tensorial method. In particular with the tensorial method, the notion of minimal conditions on A does not appear and the *Discrete Maximum Principle* is lost very fast.

1.3 Symmetry of the stencils

As we can see in Eq. (1.1) the coefficients of the approximation naturally follow the symmetries of the Laplace operator. The stencil is invariant by permutation of the axes and by symmetry with respect to any axis and to the origin.

Hence, similarly to [21], we consider the groups of points obtained by permutation π of the coordinates and symmetries S_i along the axes (Ox_i) for $1 \leq i \leq d$: *e.g.* in three dimensions $\pi_\sigma : (x_1,x_2,x_3) \mapsto (x_{\sigma(1)},x_{\sigma(2)},x_{\sigma(3)})$ with $\sigma : \{1,2,3\} \to \{1,2,3\}$ a permutation, and *e.g.* the symmetry $S_1 : (x_1,x_2,x_3) \mapsto (-x_1,x_2,x_3)$. This means for instance that $\pi(\pm 1,0,0)$ represents the following six points $(\pm 1,0,0)$, $(0,\pm 1,0)$ and $(0,0,\pm 1)$.

We plotted various two-dimensional and three-dimensional symmetric groups of points respectively in Fig. 1.1 and 1.2.

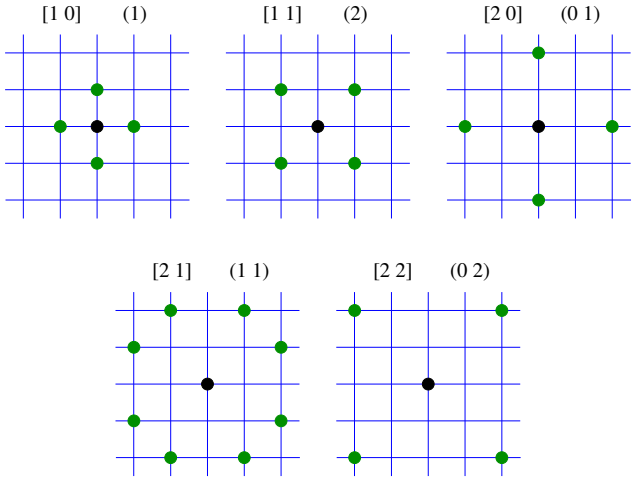


Fig. 1.1 Two-dimensional symmetric groups of points. The notation of [2] is indicated with brackets while the notation independent of the dimensionality is indicated with parenthesis.

Contrary to the notation in [2] where a symmetric group of points is denoted by the coordinates of its point which has all its coordinates positive and ordered from the largest to the smallest, we use the notation introduced in [15] called *multiplicity* and independent of the dimensionality. We denote μ the *multiplicity*. So for $\boldsymbol{\ell} \in \mathbb{N}^d$, $\mu(\boldsymbol{\ell})$ counts the number of times each non zero integer occurs as a coordinate. For instance, for $d = 4$, $\mu([2\ 1\ 1\ 0]) = (2\ 1)$. Sometimes the zeros or the

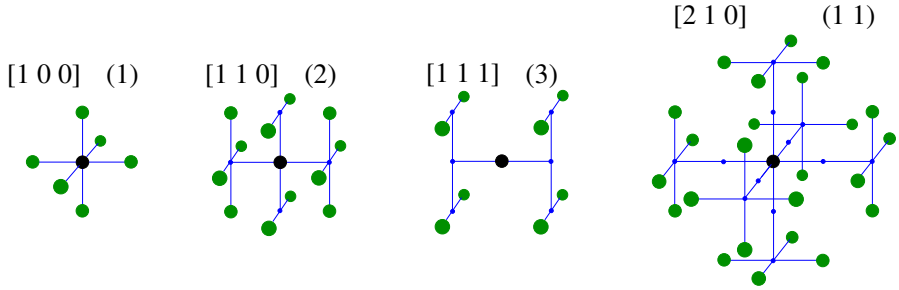


Fig. 1.2 Instances of three-dimensional symmetric groups of points with the notation from [2] on the upper left corner and the any-dimensional one on the upper right corner.

negative values are also counted, then we denote $\tilde{\mu}$ the *multiplicity* with those included, so $\tilde{\mu}([2\ 1\ 1\ 0]) = (1\ 2\ 1)$. Then we denote $\Sigma_{\mathbf{k}}$ as the group of points with k_1 coordinates equal to ± 1, k_2 coordinates equal to ± 2 and so on, that means $\mathbf{k} = \mu(\mathbf{x})$ where $\mathbf{x}$ is the denoting point from the notation [2]. So the group of points obtained by permutation of the $(\pm 2, \pm 1, \pm 1, 0)$ coordinates corresponds to $\mathbf{k} = (2,1)$. We denote $a_{\mathbf{k}}$ as the coefficient in the left-hand member of the Eqn. (0.2) associated to the $\Sigma_{\mathbf{k}}$ set and $b_{\mathbf{k}}$ the coefficient in the right-hand member associated to this same set. Hence in Eq. (0.2) we are interested in the symmetric stencils such that

$$\forall \mathbf{k}, \quad \forall \boldsymbol{\ell} \in \Sigma_{\mathbf{k}}, \quad \alpha_{\boldsymbol{\ell}} = a_{\mathbf{k}} \quad \text{and} \quad \beta_{\boldsymbol{\ell}} = b_{\mathbf{k}}.$$

Lemma 1.1 *A simple count provides the cardinality of the $\Sigma_{\mathbf{k}}$ set for $\mathbf{k} = (k_1, \ldots, k_n)$:*

$$\#(\Sigma_{\mathbf{k}}) = S_{\mathbf{k}}(1) = 2^{\mathbf{k}} \binom{d}{\mathbf{k}} \tag{1.3}$$

where

$$2^{\mathbf{k}} = 2^{\sum_{i=1}^{n} k_i} \quad \textit{and} \quad \binom{d}{\mathbf{k}} = \frac{d!}{\prod_{i=1}^{n} k_i! \, (d - \sum_{i=1}^{n} k_i)!}.$$

Proof : The number $2^{\mathbf{k}}$ corresponds to the number of sign changes in the point coordinates, $\binom{d}{\mathbf{k}}$ corresponds to the number of ways of choosing k_1 terms equal to 1 among d, then k_2 terms equal to 2 among $d - k_1$, and so on and so forth for k_i terms among $(d - k_1 - \ldots - k_{i-1})$ until i reaches n.

We denote $S_{\mathbf{k}}(1)$ as this number because –as we will see latter– it is the weight of the $\Sigma_{\mathbf{k}}$ set in the polynomial 1 when we make a Taylor expansion to the first order:

$$\sum_{\boldsymbol{\ell} \in \Sigma_{\mathbf{k}}} u(\mathbf{x} + \boldsymbol{\ell} h) = S_{\mathbf{k}}(1) u(\mathbf{x}) + O(h).$$

1.4 The Taylor series in an arbitrary dimension

The Taylor series in an arbitrary dimension d is written for $\mathbf{h} \in \mathbb{R}^d$:

$$f(\mathbf{x} + \mathbf{h}) = \sum_{p \geq 0} \frac{1}{p!} \left(\sum_{i=1}^{d} h_i \partial_i \right)^p f(\mathbf{x}) = \sum_{\boldsymbol{\lambda} \in \mathbb{N}^d} \frac{\mathbf{h}^{\boldsymbol{\lambda}}}{\boldsymbol{\lambda}!} \boldsymbol{\partial}^{\boldsymbol{\lambda}} f(\mathbf{x}) \tag{1.4}$$

with

$$\mathbf{h}^{\boldsymbol{\lambda}} = \prod_{i=1}^{d} h_i^{\lambda_i}, \quad \boldsymbol{\lambda}! = \prod_{i=1}^{d} \lambda_i! \quad \text{and} \quad \boldsymbol{\partial}^{\boldsymbol{\lambda}} = \prod_{i=1}^{d} \partial_i^{\lambda_i}.$$

This classical result is proven using the one-dimensional Taylor series. Below, as we always take the point $\mathbf{x}$ as zero, we will write f instead of $f(\mathbf{0})$.

1.5 Symmetric polynomials

In this part we use the notations from [12,20] where the interested reader could find more details about symmetric polynomials and combinatorics. As the $\Sigma_{\mathbf{k}}$ sets of points are symmetric, the Taylor series of $\sum_{\boldsymbol{\ell}\in\Sigma_{\mathbf{k}}} u(\boldsymbol{\ell}h)$ only contains terms of even degrees in ∂_i *i.e.* in Eq. (1.4) all the k_i values in $\prod_{i=1}^{d} \partial_i^{k_i}$ are even. We are able to group these polynomials in symmetric sets such as:

$$\sum_{i=1}^{d} \partial_i^2, \quad \sum_{i=1}^{d} \partial_i^4, \quad \sum_{i<j} \partial_i^2 \partial_j^2, \quad \dots$$

This drives us to consider the algebra of the symmetric polynomials noted $\mathbb{R}[s_0,\dots,s_d]$ –where (s_n) are the elementary symmetric polynomials defined underneath– for which we have known the algebraic structure since Newton's discoveries (*cf* Newton's identities).

The fundamental theorem on symmetric polynomials indicates that the following two sets of polynomials: both the set of the sums $\{\sum_{i=1}^{d} x_i^n\}_{0\le n\le d}$ and the set of the elementary symmetric polynomials $\{s_n = \sum_{i_1<i_2<\dots<i_n} \prod_{\ell=1}^{n} x_{i_\ell}\}_{0\le n\le d}$ form algebraic bases for the symmetric polynomials in dimension d.

Let $p\in\mathbb{N}$ be the degree of a polynomial, and, following [15], let $\boldsymbol{\lambda} = (\lambda_1,\lambda_2,\dots,\lambda_d)$ be a partition of p. This means that (λ_i) are integers such that $\lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_d \ge 0$ and $\sum_{i=1}^{d} \lambda_i = p$. We denote $\mathscr{P}(p)$ the set of all the partitions of $p\in\mathbb{N}$. We denote $\mathscr{S}_d$ as the set of permutations inside a set with d elements. The monomial symmetric polynomials are symmetric polynomials generated from monomials:

$$m_{\boldsymbol{\lambda}}(x_1,\dots,x_d) = \frac{1}{\tilde{\mu}(\boldsymbol{\lambda})!} \sum_{\sigma\in\mathscr{S}_d} \prod_{i=1}^{d} x_{\sigma(i)}^{\lambda_i} \tag{1.5}$$

where $\tilde{\mu}(\boldsymbol{\lambda}) = (\mu_0,\mu_1,\mu_2,\dots)$ denotes the *multiplicity* in $\boldsymbol{\lambda}$ (*cf* Part 1.3).

Theorem 1.1 (Symmetric stencil implies symmetric Taylor expansion) *Let $\Sigma_{[\boldsymbol{x}]}$ denote the group of points obtained by permutation of the coordinates of the point $\boldsymbol{x} = (x_1,x_2,\dots,x_d)\in\mathbb{Z}^d$. Then the Taylor expansion of*

$$\sum_{\boldsymbol{\ell}\in\Sigma_{[\boldsymbol{x}]}} u(\boldsymbol{\ell}h) = \frac{1}{\tilde{\mu}(\boldsymbol{x})!} \sum_{\sigma\in\mathscr{S}_d} u(x_{\sigma(1)}h, x_{\sigma(2)}h, \dots, x_{\sigma(d)}h)$$

is expressed in the basis of the symmetric monomials $(m_{\boldsymbol{\lambda}})_{\boldsymbol{\lambda}\in\mathscr{P}(p),p\ge 0}$ as

$$\sum_{\boldsymbol{\ell}\in\Sigma_{[\boldsymbol{x}]}} u(\boldsymbol{\ell}h) = \sum_{p\ge 0} h^p \sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)} \frac{\tilde{\mu}(\boldsymbol{\lambda})!}{\boldsymbol{\lambda}!\tilde{\mu}(\boldsymbol{x})!} m_{\boldsymbol{\lambda}}(\boldsymbol{x}) m_{\boldsymbol{\lambda}}(\partial_1,\dots,\partial_d) u. \tag{1.6}$$

Proof: This can be proved by direct computation thanks to Taylor expansion and permutation of the sums and of the permutation operators.

$$\begin{aligned}
\sum_{\boldsymbol{\ell}\in\Sigma_{[\mathbf{x}]}} u(\boldsymbol{\ell}h) &= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{\sigma\in\mathscr{S}_d}\sum_{p\geq 0}\frac{h^p}{p!}\left(\sum_{i=1}^d x_{\sigma(i)}\partial_i\right)^p u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}\frac{h^p}{p!}\sum_{\sigma\in\mathscr{S}_d}\left(\sum_{i=1}^d x_i\partial_{\sigma^{-1}(i)}\right)^p u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}\frac{h^p}{p!}\sum_{\sigma\in\mathscr{S}_d}\left(\sum_{i=1}^d x_i\partial_{\sigma(i)}\right)^p u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}\frac{h^p}{p!}\sum_{\sigma\in\mathscr{S}_d}\sum_{\substack{\mathbf{q}\in\mathbb{N}^d\\|\mathbf{q}|_1=p}}\binom{p}{\mathbf{q}}\prod_{i=1}^d x_i^{q_i}\partial_{\sigma(i)}^{q_i}u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}\frac{h^p}{p!}\sum_{\sigma\in\mathscr{S}_d}\sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)}\frac{1}{\tilde{\mu}(\boldsymbol{\lambda})!}\sum_{\tau\in\mathscr{S}_d}\binom{p}{\boldsymbol{\lambda}\circ\tau}\prod_{i=1}^d x_i^{\lambda_{\tau(i)}}\partial_{\sigma(i)}^{\lambda_{\tau(i)}}u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}h^p\sum_{\sigma\in\mathscr{S}_d}\sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)}\frac{1}{\tilde{\mu}(\boldsymbol{\lambda})!\boldsymbol{\lambda}!}\sum_{\tau\in\mathscr{S}_d}\prod_{i=1}^d x_{\tau(i)}^{\lambda_i}\partial_{\sigma\circ\tau(i)}^{\lambda_i}u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}h^p\sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)}\frac{1}{\tilde{\mu}(\boldsymbol{\lambda})!\boldsymbol{\lambda}!}\sum_{\tau\in\mathscr{S}_d}\sum_{\sigma\in\mathscr{S}_d}\prod_{i=1}^d x_{\tau(i)}^{\lambda_i}\partial_{\sigma(i)}^{\lambda_i}u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}h^p\sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)}\frac{1}{\tilde{\mu}(\boldsymbol{\lambda})!\boldsymbol{\lambda}!}\left(\sum_{\tau\in\mathscr{S}_d}\prod_{i=1}^d x_{\tau(i)}^{\lambda_i}\right)\left(\sum_{\sigma\in\mathscr{S}_d}\prod_{i=1}^d\partial_{\sigma(i)}^{\lambda_i}\right)u \\
&= \frac{1}{\tilde{\mu}(\boldsymbol{x})!}\sum_{p\geq 0}h^p\sum_{\boldsymbol{\lambda}\in\mathscr{P}(p)}\frac{\tilde{\mu}(\boldsymbol{\lambda})!}{\boldsymbol{\lambda}!}m_{\boldsymbol{\lambda}}(\boldsymbol{x})m_{\boldsymbol{\lambda}}(\boldsymbol{\partial})u.
\end{aligned}$$

Further in Lemma 1.2 we derive an equivalent expression in the special case of an additional $\pm$ symmetry (hence the $2^{\mathbf{k}}$ factor and the exclusive even degree) to express the Taylor expansion of the stencils $\Sigma_{\mathbf{k}}$ in the basis of the monomials of even degrees.

In Table 1.1, we list all the symmetric monomials according to their degree p. Their cardinality is indicated in the last row and provides the number of equations that coefficients $(a_{\mathbf{k}})$ and $(b_{\mathbf{k}})$ have to satisfy for each elevation of order. A new column p is formed by considering the first number q going from p to 1, then completing it with the groups starting at the most by q in the column $p-q$. This table can also be found in the textbook [20] p287.

The symmetric monomials have the property that their multiplication does not depend on the dimensionality. For instance, for any $d\geq 2$, we have $m_{\mathbf{1}}^2 = m_{\mathbf{2}} + 2m_{\mathbf{11}}$ which stands for

$$\left(\sum_{i=1}^d x_i\right)^2 = \sum_{i=1}^d x_i^2 + 2\sum_{i<j} x_i x_j.$$

Table 1.1 A summary table of all the monomial symmetric polynomials $m_{\boldsymbol{\lambda}}$ of degree inferior or equal to 5 in an arbitrary dimension. A finite dimension d restricts the number of terms in a group to d.

degree p	0	1	2	3	4	5
indices $\boldsymbol{\lambda}$ in the polynomials $m_{\boldsymbol{\lambda}}$	$\emptyset$	**1**	**2** **11**	**3** **21** **111**	**4** **31** **22** **211** **1111**	**5** **41** **32** **311** **221** **2111** **11111**
#	1	1	2	3	5	7

We will use symmetric polynomials for $x_i = \partial_i^2$, $1 \leq i \leq d$.

Their cardinality is independent from the dimension, and relatively moderate compared to all the polynomials appearing in the Taylor series (1.4). This allows that when we write Eq. (0.2) in the vectorial basis of the symmetric even monomial polynomials noted $(m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2}))$ short for $(m_{\boldsymbol{\lambda}}(\partial_1^2,\dots,\partial_d^2))$, we obtain:

$$\frac{1}{h^2}\sum_{\lambda_1\geq\cdots\geq\lambda_d\geq 0} c_{\boldsymbol{\lambda}}^u \frac{h^{2|\boldsymbol{\lambda}|}}{(2\boldsymbol{\lambda})!} m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})\,u = \sum_{\lambda_1\geq\cdots\geq\lambda_d\geq 0} c_{\boldsymbol{\lambda}}^v \frac{h^{2|\boldsymbol{\lambda}|}}{(2\boldsymbol{\lambda})!} m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})\,v \qquad (1.7)$$

with $|\boldsymbol{\lambda}| = \sum_{i=1}^n \lambda_i$. Replacing the coefficients $c_{\boldsymbol{\lambda}}^u$ and $c_{\boldsymbol{\lambda}}^v$ by their respective expressions $\sum_{\mathbf{k}} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}})a_{\mathbf{k}}$ and $\sum_{\mathbf{k}} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}})b_{\mathbf{k}}$ and taking v as $\Delta u = m_{\mathbf{1}}(\boldsymbol{\partial^2})\,u$, we solve the system of equations formed on the coefficients $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$:

$$\sum_{\lambda_1\geq\cdots\geq\lambda_d\geq 0}\left(\sum_{\mathbf{k}\in\{0,\dots,d\}^n} a_{\mathbf{k}} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2}))\right)\frac{m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})\,u}{(2\boldsymbol{\lambda})!}$$

$$= \sum_{\lambda_1\geq\cdots\geq\lambda_d\geq 0}\left(\sum_{\mathbf{k}\in\{0,\dots,d\}^n} b_{\mathbf{k}} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2}))\right)\frac{m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})m_{\mathbf{1}}(\boldsymbol{\partial^2})\,u}{(2\boldsymbol{\lambda})!} \qquad (1.8)$$

with $S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2}))$ being coefficients that we are going to explicitly compute in Eq. (1.9). To simplify, as it does not play any role, in Eq. (1.8) we consider $h = 1$.

1.6 Taylor series of the sums on $\Sigma_{\mathbf{k}}$ expressed in the symmetric polynomials basis

For $\Sigma_{\mathbf{k}}$ a given symmetric group of points with $\mathbf{k}$ a tuple of integers, we aim to express the Taylor series $\sum_{\boldsymbol{\ell}\in\Sigma_{\mathbf{k}}} u(\boldsymbol{\ell}h)$ with the help of the symmetric polynomials. If we denote $m_{\boldsymbol{\lambda}}$ as the symmetric monomial which contains $x_1^{\lambda_1}\dots x_d^{\lambda_d}$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0$ then

$$\sum_{\boldsymbol{\ell}\in\Sigma_{\mathbf{k}}} u(\boldsymbol{\ell}h) = \sum_{\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_d\geq 0} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\partial_1^2,\dots,\partial_d^2))\frac{h^{2\boldsymbol{\lambda}}}{(2\boldsymbol{\lambda})!} m_{\boldsymbol{\lambda}}(\partial_1^2,\dots,\partial_d^2)u,$$

with the $S_{\mathbf{k}}(m_{\boldsymbol{\lambda}})$ values given by the following lemma:

Lemma 1.2 *For $1 \le n \le d$ and $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 1$ the computation of $S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2}))$ is given by the formula:*

$$\begin{aligned} S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\partial_1^2,\dots,\partial_d^2)) &= S_{\mathbf{k}}(\partial_1^{2\lambda_1}\dots\partial_n^{2\lambda_n}) \\ &= 2^{\mathbf{k}} \sum_{i_1=1}^{q} \cdots \sum_{i_n=1}^{q} \left(\prod_{r=1}^{n} i_r^{2\lambda_r}\right) \binom{d-n}{\mathbf{k}-\mu(\boldsymbol{i})}, \end{aligned} \tag{1.9}$$

with $q \in \mathbb{N}$, $\mathbf{k} = (k_1, k_2, \dots, k_q)$ and with $\binom{d-n}{\mathbf{k}-\mu(\boldsymbol{i})}$ equal to zero if one of the terms $d-n$, $k_\ell - \mu_\ell(\boldsymbol{i})$ for $1 \le \ell \le q$ or $d-n-\sum_\ell (k_\ell - \mu_\ell(\boldsymbol{i}))$ is strictly negative.

Proof: For $i_1, i_2, \dots, i_n \ge 1$ being given, we count the number of points of $\Sigma_{\mathbf{k}}$ which are of the type $(\pm i_1, \pm i_2, \dots, \pm i_n, i_{n+1}, \dots, i_d)$ i.e. which have a factor $\prod_{r=1}^{n} i_r^{2\lambda_r}$ in front of the partial derivative $\partial_1^{2\lambda_1}\dots\partial_n^{2\lambda_n}$ in their Taylor series. $2^{\mathbf{k}}$ possibilities are offered by the sign changes, and for each value of $\ell \ge 1$, $k_\ell - \#\{r, i_r = \ell\}$ terms equal to ℓ remains and have to be placed in the $d-n$ coordinates $(i_{n+1}, \dots, i_d)$. Hence, we obtain this particularly useful expression, which can be easily implemented and allows an automatic computation of the coefficients $S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}(\partial_1^2,\dots,\partial_d^2))$. The $n = 0$ case corresponding to $m_\emptyset = 1$ is given by Lemma 1.1.

1.7 Identification of the terms for the equation $\Delta u = v$

To identify the terms of the Taylor series

$$\frac{1}{h^2}\sum_{\mathbf{k}} a_{\mathbf{k}} \sum_{\boldsymbol{\ell}\in\Sigma_{\mathbf{k}} h} u(\boldsymbol{\ell}h) = \frac{1}{h^2} \sum_{\lambda_1\ge\cdots\ge\lambda_d\ge 0} c_{\boldsymbol{\lambda}}^{u} \frac{h^{2|\boldsymbol{\lambda}|}}{(2\boldsymbol{\lambda})!} m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})\, u \tag{1.10}$$

and

$$\sum_{\mathbf{k}} b_{\mathbf{k}} \sum_{\boldsymbol{\ell}\in\Sigma_{\mathbf{k}} h} v(\boldsymbol{\ell}h) = \sum_{\lambda_1\ge\cdots\ge\lambda_d\ge 0} c_{\boldsymbol{\lambda}}^{v} \frac{h^{2|\boldsymbol{\lambda}|}}{(2\boldsymbol{\lambda})!} m_{\boldsymbol{\lambda}}(\boldsymbol{\partial^2})\, v \tag{1.11}$$

using symmetric polynomials, we replace v by $\Delta u = m_{\mathbf{1}}(\partial_1^2,\dots,\partial_d^2)u = \sum_{i=1}^{d}\partial_i^2 u$ in its Taylor series. This is equivalent to multiplying each symmetric polynomial on the right-hand side of Eq. (1.11) by $m_{\mathbf{1}} = \sum_{i=1}^{d}\partial_i^2$.

In Table 1.2 we identify the equalities between the terms of the symmetric Taylor series on u and the terms of the symmetric Taylor series on v. The symmetric polynomials issued from v are multiplied by $m_{\mathbf{1}}$ in a way that is independent from the dimensionality. The symmetric polynomials coefficients $c_{\boldsymbol{\lambda}}^{v}$ of the Taylor series on v are set in front to those of u with, next to them, the multiplication factors: the one coming from the multiplication by $m_{\mathbf{1}}$ and the one coming from the Taylor expansion coefficient $\frac{1}{(2\boldsymbol{\lambda})!}$.

Hence, each row corresponds to a condition applying to the coefficients $(a_{\mathbf{k}})$ and $(b_{\mathbf{k}})$, knowing that if the number of components of a symmetric polynomial in a row exceeds the dimensionality, it disappears. As a result, including the normalization condition (*cf* Theorem 1.2), in dimension three, 17 equations are required to reach the 10th order.

Table 1.2 Table summarizing the conditions on the coefficients $c^u_{\boldsymbol{\lambda}}$ and $c^v_{\boldsymbol{\lambda}}$ in front of the symmetric polynomials $m_{\boldsymbol{\lambda}}$ in the Taylor series for u and v in (1.7) with their various factors.

$(2\boldsymbol{\lambda})!$	$\boldsymbol{\lambda}(u)$	$m_{\mathbf{1}}\times$	$\boldsymbol{\lambda}(v)$	$(2\boldsymbol{\lambda}(u))!/(2\boldsymbol{\lambda}(v))!$
	2nd order		$m_{\mathbf{1}}\times m_{\emptyset}=m_{\mathbf{1}}$	
1	u		0	
2	**1**		v	2
	4th order		$m_{\mathbf{1}}\times m_{\mathbf{1}}=m_{\mathbf{2}}+2m_{\mathbf{11}}$	
4!	**2**		**1**	12
4	**11**	$\times 2$	**1**	2
	6th order		$m_{\mathbf{1}}\times m_{\mathbf{2}}=m_{\mathbf{3}}+m_{\mathbf{21}}$ $m_{\mathbf{1}}\times m_{\mathbf{11}}=m_{\mathbf{21}}+3m_{\mathbf{111}}$	
6!	**3**		**2**	30
$2\cdot 4!$	**21**		**2+11**	2+12
8	**111**	$\times 3$	**11**	2
	8th order		$m_{\mathbf{1}}\times m_{\mathbf{3}}=m_{\mathbf{4}}+m_{\mathbf{31}}$ $m_{\mathbf{1}}\times m_{\mathbf{21}}=m_{\mathbf{31}}+2m_{\mathbf{22}}+2m_{\mathbf{211}}$ $m_{\mathbf{1}}\times m_{\mathbf{111}}=m_{\mathbf{211}}+4m_{\mathbf{1111}}$	
8!	**4**		**3**	56
$2\cdot 6!$	**31**		**3+21**	2+30
$4!^2$	**22**	$\times 2$	**21**	12
$4\cdot 4!$	**211**		$\underbrace{\mathbf{21}}_{\times 2}+\mathbf{111}$	2+12
2^4	**1111**	$\times 4$	**111**	2
	10th order		$m_{\mathbf{1}}\times m_{\mathbf{4}}=m_{\mathbf{5}}+m_{\mathbf{41}}$ $m_{\mathbf{1}}\times m_{\mathbf{31}}=m_{\mathbf{32}}+m_{\mathbf{41}}+2m_{\mathbf{311}}$ $m_{\mathbf{1}}\times m_{\mathbf{22}}=m_{\mathbf{32}}+m_{\mathbf{221}}$ $m_{\mathbf{1}}\times m_{\mathbf{211}}=m_{\mathbf{311}}+2m_{\mathbf{221}}+3m_{\mathbf{2111}}$ $m_{\mathbf{1}}\times m_{\mathbf{1111}}=m_{\mathbf{2111}}+5m_{\mathbf{11111}}$	
10!	**5**		**4**	90
$2\cdot 8!$	**41**		**4+31**	2+56
$6!\cdot 4!$	**32**		**31+22**	12+30
$6!\cdot 4$	**311**		$\underbrace{\mathbf{31}}_{\times 2}+\mathbf{211}$	2+30
$4!^2\cdot 2$	**221**		$\mathbf{22}+\underbrace{\mathbf{211}}_{\times 2}$	2+12
$8\cdot 4!$	**2111**		$\underbrace{\mathbf{211}}_{\times 3}+\mathbf{1111}$	2+12
2^5	**11111**	$\times 5$	**1111**	2

For instance, the first row corresponds to $\boldsymbol{\lambda}(u)=\emptyset$ *i.e.* to the sum of the coefficients applied to u:

$$\sum_{\mathbf{k}} S_{\mathbf{k}}(1)a_{\mathbf{k}}=0. \tag{1.12}$$

The second row, as $m_{\mathbf{1}}\times m_{\emptyset}=m_{\mathbf{1}}$, provides:

$$\sum_{\mathbf{k}} S_{\mathbf{k}}(\partial_1^2)a_{\mathbf{k}}=2\sum_{\mathbf{k}} S_{\mathbf{k}}(1)b_{\mathbf{k}}.$$

For the following rows we observed that $m_{\mathbf{1}} \times m_{\mathbf{1}} = m_{\mathbf{2}} + 2m_{\mathbf{11}}$ independently of the dimension, hence we deduce the third row:

$$\sum_{\mathbf{k}} S_{\mathbf{k}} (\partial_1^4) a_{\mathbf{k}} = 12 \sum_{\mathbf{k}} S_{\mathbf{k}} (\partial_1^2) b_{\mathbf{k}},$$

and the fourth row:

$$\sum_{\mathbf{k}} S_{\mathbf{k}} (\partial_1^2 \partial_2^2) a_{\mathbf{k}} = 4 \sum_{\mathbf{k}} S_{\mathbf{k}} (\partial_1^2) b_{\mathbf{k}}.$$

This allows us to state the main result of this manuscript:

Theorem 1.2 (Arbitrary order of the Mehrstellenverfahren scheme in an arbitrary dimension) *Let the coefficients $(a_{\mathbf{k}})$ and $(b_{\mathbf{k}})$ satisfy both the equations induced by Table 1.2 and its continuation until a given arbitrary order and:*

$$\sum_{\mathbf{k}} S_{\mathbf{k}} (\sum_{i=1}^{d} \partial_i^2) a_{\mathbf{k}} \neq 0, \tag{1.13}$$

with the coefficients $S_{\mathbf{k}}$ defined in Lemmas 1.1 and 1.2. In Eq. (0.2), they form a compact finite difference scheme of arbitrary order in an arbitrary dimension to solve the Poisson equation $\Delta u = v$ on a uniform Cartesian grid.

Proof: This theorem follows on from what was explained previously. The functions u and v are supposed to be very smooth so that the sums (1.10) and (1.11) are developed in the Taylor series for which we regroup the derivatives in monomial symmetric polynomials in ∂_i^2.

The identification of these developments is given in Table 1.2. If all the conditions are satisfied then the residual is of degree 12 in h, which divided by h^2 provides a 10th order. The rows of this table may be continued, to reach higher orders.

To solve $\Delta u = v$ and discard the $1/h^2 Au = O(h^2) = Bv$ for all functions u and v case, we add the condition Eq. (1.13) that guarantees that $1/h^2 Au = K\Delta u + O(h^2) = Kv + O(h^2) = Bv$ with $K \neq 0$. In this whole manuscript, we normalize the coefficients to obtain $K = 1$.

2 Computation of the coefficients in particular cases

Before computing new high order schemes, we reviewed various previously published compact finite difference schemes on uniform Cartesian grids [1,3,11,17,19, 21,22]. Theorem 1.2 allows these schemes to be recovered.

2.1 Compact finite difference Poisson solvers extracted from the literature

2.1.1 Sixth order schemes in dimension two

For $d = 2$, we compare the results of the present method with the compact finite difference approximations introduced in [3,1,22] back to years 1951, 1953 and 1980

respectively. The coefficients a_0, a_1, a_2, b_0, b_1, b_2 and b_{01} correspond to the symmetric stencils respectively associated to $\alpha_{[0\ 0]}$, $\alpha_{[1\ 0]}$, $\alpha_{[1\ 1]}$, $\beta_{[0\ 0]}$, $\beta_{[1\ 0]}$, $\beta_{[1\ 1]}$ and $\beta_{[2\ 0]}$ if we apply for the Greek letters a notation consistent with the one used in [2]. These stencils are represented in Fig. 1.1 where the correspondence between the two notations is indicated. Then the first seven rows of Table 1.2 provide the six equations concerning $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ coefficients:

$$a_0 + 4*a_1 + 4*a_2 = 0 \tag{2.1}$$
$$a_1 + 2*a_2 = b_0 + 4*b_1 + 4*b_2 + 4*b_{01} \tag{2.2}$$
$$a_1 + 2*a_2 = 12*b_1 + 24*b_2 + 48*b_{01} \tag{2.3}$$
$$a_2 = 2*b_1 + 4*b_2 + 8*b_{01} \tag{2.4}$$
$$a_1 + 2*a_2 = 30*b_1 + 60*b_2 + 480*b_{01} \tag{2.5}$$
$$a_2 = b_1 + 14*b_2 + 16*b_{01}. \tag{2.6}$$

We add the equation corresponding to $1/h^2 A\,u = \Delta u + O(h^2)$ to these to be sure that we solve the Poisson equation:

$$a_1 + 2*a_2 = 1. \tag{2.7}$$

This normalizes the coefficients.

Eqns. (2.1), (2.3)$-6\times$(2.4) and (2.7) imply:

$$a_0 = -\frac{10}{3}, \quad a_1 = \frac{2}{3}, \quad a_2 = \frac{1}{6}.$$

Next comes:

$$b_0 = \frac{119}{180}, \quad b_1 = \frac{7}{90}, \quad b_2 = \frac{1}{90}, \quad b_{01} = -\frac{1}{240}.$$

We can visualize this scheme as follows:

$$\frac{1}{6h^2}\begin{array}{ccc} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{array} u = \frac{1}{720}\begin{array}{ccccc} & & -3 & & \\ & 8 & 56 & 8 & \\ -3 & 56 & 476 & 56 & -3 \\ & 8 & 56 & 8 & \\ & & -3 & & \end{array} v. \tag{2.8}$$

We see that if $v = 0$, we can solve the Laplace equation $\Delta u = 0$ at the sixth order, whereas for any regular function f, the Δf approximation Af without perturbation is only second order.

If instead of b_{01} we had activated a_{01}, we would have obtained the scheme presented in the appendix of the book by L. Collatz [3] p 543:

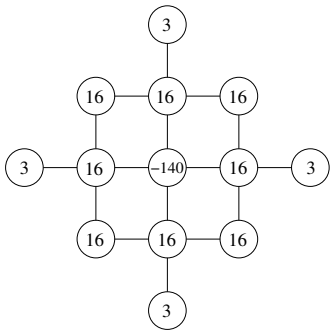
$$a_0 = -\frac{7}{3}, \quad a_1 = \frac{4}{15}, \quad a_2 = \frac{4}{15}, \quad a_{01} = \frac{1}{20}$$

and

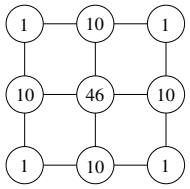
$$b_0 = \frac{23}{45}, \quad b_1 = \frac{1}{9}, \quad b_2 = \frac{1}{90}.$$

This scheme can be visualized as follows:

$$\frac{1}{60h^2}$$



$$u = \frac{1}{90}$$



$$v. \qquad (2.9)$$

2.1.2 Sixth order scheme in dimension three: the HOC Stencil

For $d = 3$, if we activate the coefficients a_0, a_1, a_2, a_3, b_0, b_1, b_2, b_3 and b_{01}, the first seven rows of Table 1.2 give the equations:

$$\begin{aligned}
a_0 + 6*a_1 + 12*a_2 + 8*a_3 &= 0 \\
a_1 + 4*a_2 + 4*a_3 &= b_0 + 6*b_1 + 12*b_2 + 8*b_3 + 6*b_{01} \\
a_1 + 4*a_2 + 4*a_3 &= 12*b_1 + 48*b_2 + 48*b_3 + 48*b_{01} \\
a_2 + 2*a_3 &= 2*b_1 + 8*b_2 + 8*b_3 + 8*b_{01} \\
a_1 + 4*a_2 + 4*a_3 &= 30*b_1 + 120*b_2 + 120*b_3 + 480*b_{01} \\
a_2 + 2*a_3 &= b_1 + 16*b_2 + 28*b_3 + 16*b_{01} \\
a_3 &= 3*b_2 + 6*b_3.
\end{aligned}$$

To these we add the normalization equation

$$a_1 + 4*a_2 + 4*a_3 = 1.$$

Then, the general solution of this system is given by:

$$a_0 = -\frac{64}{15}, \quad a_1 = \frac{7}{15}, \quad a_2 = \frac{1}{10}, \quad a_3 = \frac{1}{30}, \qquad (2.10)$$

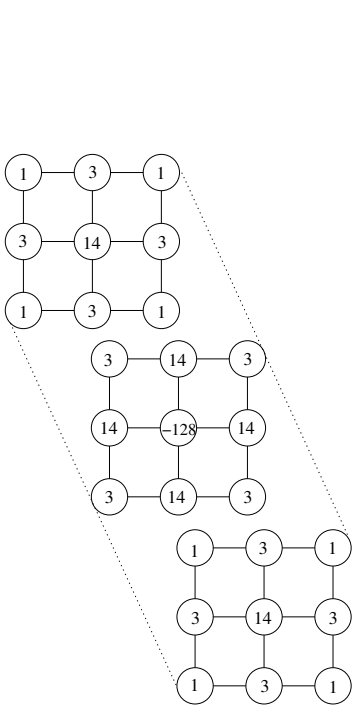
and we obtain:

$$b_0 = -8*\beta + \frac{67}{120},\ b_1 = 4*\beta + \frac{1}{18},\ b_2 = -2*\beta + \frac{1}{90},\ b_3 = \beta,\ b_{01} = -\frac{1}{240} \qquad (2.11)$$

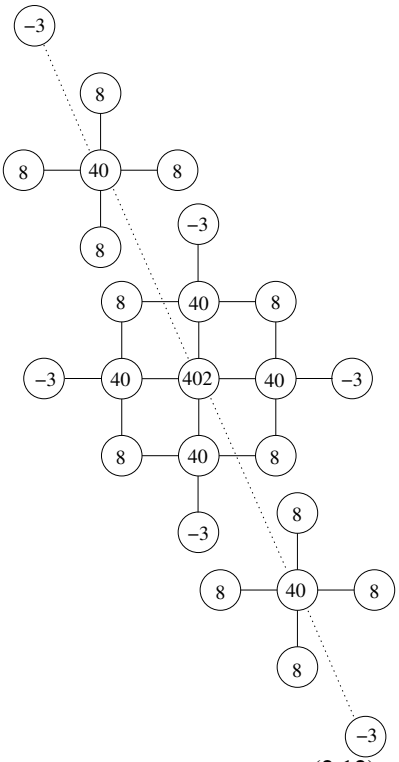
for any $\beta \in \mathbb{R}$.

With $\beta = 0$ this three dimensional scheme can be visualized as:

$$\frac{1}{30h^2}$$



$$u = \frac{1}{720}$$



$$v. \tag{2.12}$$

This scheme was introduced in [19], at least regarding $(a_{\mathbf{k}})$ and then extended with the addition of $(b_{\mathbf{k}})$ and tested in [21].

2.1.3 Fourth order scheme in an arbitrary dimension

In an arbitrary dimension, the fourth order is provided by the first four rows of Table 1.2, that is for $\boldsymbol{\lambda}(u) = \emptyset, \mathbf{1}, \mathbf{2}$ and $\mathbf{11}$.
If we only activate the first rank of $\mathbf{k}$, $\mathbf{k} = (k_1) = (k)$, then for the symmetric monomial $m_{\boldsymbol{\lambda}}$ containing $\partial_1^{2\lambda_1} \dots \partial_n^{2\lambda_n}$ (case $\mathbf{i} = (\underbrace{1, \dots, 1}_{n \text{ times}})$ in Eq. (1.9)),

$$S_k(m_{\boldsymbol{\lambda}}) = S_k^n = 2^k \binom{d-n}{k-n}. \tag{2.13}$$

Table 1.2 provides the equations

$$\sum_{k=0}^{d} S_k^0 a_k = 0, \tag{2.14}$$

$$\sum_{k=1}^{d} S_k^1 a_k = 2 \sum_{k=0}^{d} S_k^0 b_k = 2, \tag{2.15}$$

$$\sum_{k=1}^{d} S_k^1 a_k = 12 \sum_{k=1}^{d} S_k^1 b_k, \tag{2.16}$$

$$\sum_{k=2}^{d} S_k^2 a_k = 4 \sum_{k=1}^{d} S_k^1 b_k. \tag{2.17}$$

Hence the coefficients (a_k) are given by the equations:

$$\sum_{k=0}^{d} S_k^0 a_k = 0, \quad \sum_{k=1}^{d} S_k^1 a_k = 2, \quad \sum_{k=2}^{d} S_k^2 a_k = \frac{2}{3}.$$

If we activate the coefficients a_0, a_1, a_2, a_d, we need to compute the following values of (S_k^n):

$$S_0^0 = 1, \quad S_1^0 = 2d, \quad S_2^0 = 2d(d-1), \quad S_d^0 = 2^d, \quad S_0^1 = 0,$$
$$S_1^1 = 2, \quad S_2^1 = 4(d-1), \quad S_d^1 = 2^d, \quad S_2^2 = 4, \quad S_d^2 = 2^d.$$

Then the equations (2.18) become:

$$\begin{cases} a_0 + 2d\,a_1 + 2d(d-1)\,a_2 + 2^d\,a_d = 0 \\ 2\,a_1 + 4(d-1)\,a_2 + 2^d\,a_d = 2 \\ 4\,a_2 + 2^d\,a_d = \frac{2}{3} \end{cases} .$$

For $a_d = 0$, we find the scheme presented in the book by Samarskii [17] p297 with varying mesh sizes depending on the direction. Provided they are taken back to the uniform grid, they are given by:

$$a_0 = \frac{d(d-7)}{3}, \quad a_1 = \frac{4-d}{3}, \quad a_2 = \frac{1}{6}.$$

Then the coefficients (b_k) have to satisfy:

$$\sum_{k=0}^{d} S_k^0 b_k = 1, \quad \sum_{k=1}^{d} S_k^1 b_k = \frac{1}{6}.$$

Activating the coefficients b_0 and b_1, we obtain the equations:

$$\begin{cases} b_0 + 2d\,b_1 = 1 \\ 2\,b_1 = \frac{1}{6} \end{cases}$$

for which the solution is:

$$b_0 = \frac{6-d}{6}, \quad b_1 = \frac{1}{12}.$$

The trouble with such a scheme is that for $d \geq 4$, $a_1 \leq 0$ which hampers the use of an iterative solver of the Gauss-Seidel type.

If we take $a_2 = 0$ in Eq. (2.18), we find the following scheme extracted from the book by Iserles [17] (exercise 7.11 p134):

$$a_0 = -\frac{2(2d+1)}{3}, \quad a_1 = \frac{2}{3}, \quad a_d = \frac{1}{3 \cdot 2^{d-1}}.$$

It circumvents the problem of the previous scheme since whatever the value of d, its only strictly negative coefficient is a_0. The same previous conditions apply to the coefficients (b_k) so we can take

$$b_0 = \frac{6-d}{6}, \quad b_1 = \frac{1}{12}.$$

2.2 Minimal conditions on the coefficients $(a_{\mathbf{k}})$ of the operator A

Finding the minimal conditions that the coefficients $(a_{\mathbf{k}})$ have to satisfy independently of the coefficients $(b_{\mathbf{k}})$ corresponds to the design of a discrete solver for the Laplace equation: $\Delta u = 0$ [11].

Let $x_i = \partial_i^2$ and $(s_i)_{0 \leq i \leq d}$ denote the elementary symmetric polynomials defined in Part 1.5. If we assume that in Eq. (1.8) the right-hand member generates $s_1 \mathbb{R}[s_0, \ldots, s_d]$ and the left-hand member $\mathbb{R}[s_0, \ldots, s_d]$, we deduce the monomials that impose strict conditions on the coefficients $(a_{\mathbf{k}})$: $s_0 = m_{\emptyset} = \mathbf{1}$, $s_2 = m_{\mathbf{11}}$, $s_3 = m_{\mathbf{111}}$ until $s_d = m_{\mathbf{1 \ldots 1}}$ with as many $\mathbf{1}$'s as there are dimensions plus the algebra they generate, hence including $m_{\mathbf{11}}^2$, $m_{\mathbf{11}} m_{\mathbf{111}}$ etc.

First of all, there is one condition owing on $(a_{\mathbf{k}})$ from $Au = h^2 \Delta u + o(h^3)$ for any smooth function u. Hence in dimension two, there are two conditions acting on the coefficients $(a_{\mathbf{k}})$ to reach the second order (including the one imposed by $\mathbf{1}$), three for the 4th and 6th orders (including the one imposed by $m_{\mathbf{11}}$) and four for the 8th and 10th orders (adding $m_{\mathbf{11}}^2$). In contrast, in dimension three there are two conditions for the second order (from $\mathbf{1}$ and $m_{\mathbf{1}}$), three for the fourth order (addition of $m_{\mathbf{11}}$), four for the 6th order (addition of $m_{\mathbf{111}}$), five for the 8th order (addition of $m_{\mathbf{11}}^2$) and six for the 10th order (addition of $m_{\mathbf{11}} m_{\mathbf{111}}$).

In practice, we eliminate the $c_{\boldsymbol{\lambda}}^v$ terms from the equations of Table 1.2 by linear combinations of the lines so we obtain conditions only on $c_{\boldsymbol{\lambda}}^u$.

Then depending on which $a_{\mathbf{k}}$ points we choose to activate, these conditions vary. When we solve the system, the number of indices $\mathbf{k}$ for which $a_{\mathbf{k}}$ are activated is taken equal to the number of linear equations. In dimension two, the activation of the first rank ($\mathbf{k}$ has only one component k_1) allows the 6th order to be reached. The associated conditions are given for the second order by:

$$a_0 + 4a_1 + 4a_2 = 0,$$

$$a_1 + 2a_2 = 1$$

and for the fourth and sixth orders by:

$$a_1 - 4a_2 = 0.$$

The activation of the second rank allows the sixth order to be passed and the 18th order to be reached (see Part 2.4). The conditions for the second order become:

$$a_0+4a_1+4a_2+4a_{01}+8a_{11}+4a_{02}=0, \tag{2.18}$$

$$a_1+2a_2+4a_{01}+10a_{11}+8a_{02}=1. \tag{2.19}$$

To which, for the 4th and 6th orders we have to add:

$$a_1-4a_2+16a_{01}-14a_{11}-64a_{02}=0. \tag{2.20}$$

To reach the 8th and 10th orders, we also have to add:

$$a_1+16a_2+256a_{01}-1054a_{11}+4096a_{02}=0. \tag{2.21}$$

These equations produce the 10th order schemes presented and tested in [22] for the Laplace equation.

In dimension three, if we only activate the coefficients $\mathbf{k}=(k_1)$ of the first rank, we reach the second order under the conditions:

$$a_0+6a_1+12a_2+8a_3=0,$$

$$a_1+4a_2+4a_3=1,$$

the fourth order by adding:

$$a_1-2a_2-8a_3=0$$

and the sixth order thanks to:

$$a_1-26a_2+64a_3=0.$$

If these three conditions are verified, we find the *HOC Stencil* from [19], see section 2.1.2.

If we now activate all the points of the first and second ranks $\mathbf{k}=(k_1,k_2)$, we obtain the four conditions:

$$a_0+6a_1+12a_2+8a_3+6a_{01}+24a_{11}+24a_{21}+12a_{02}+24a_{12}+8a_{03}=0, \tag{2.22}$$

$$a_1+4a_2+4a_3+4a_{01}+20a_{11}+24a_{21}+16a_{02}+36a_{12}+16a_{03}=1, \tag{2.23}$$

$$a_1-2a_2-8a_3+16a_{01}+20a_{11}-36a_{21}-32a_{02}-156a_{12}-128a_{03}=0, \tag{2.24}$$

$$a_1-26a_2+64a_3+64a_{01}-340a_{11}+444a_{21}-1664a_{02}+1236a_{12}+4096a_{03}=0. \tag{2.25}$$

To reach the 8th order, we have to add to these conditions:

$$a_1+18a_2+32a_3+256a_{01}-540a_{11}-2076a_{21}+4608a_{02}+6084a_{12}+8192a_{03}=0 \tag{2.26}$$

and to reach the 10th order:

$$a_1 - 2a_2 - 512a_3 + 1024a_{01} - 12580a_{11} + 25164a_{21} - 2048a_{02} + 59316a_{12} - 524288a_{03} = 0. \tag{2.27}$$

We still need to determine the coefficients $(b_{\mathbf{k}})$ whose distribution area should be much wider than that of $(a_{\mathbf{k}})$.

The following theorem indicates that even if the number of $a_{(k_1)}$ coefficients for $0 \leq k_1 \leq d$ increases with the number of dimensions (d), while the number of equations they have to satisfy stays still, the order of the compact solver $Au = Bv$ is limited to the sixth one as long as we only activate the first rank $\mathbf{k} = (k_1)$ coefficients in A.

Theorem 2.1 (maximal sixth order for the strictly compact finite difference schemes) *For $d \geq 2$ any numerical scheme for the Poisson equation relying on a symmetric strictly compact finite difference scheme, which means whose $(a_{\mathbf{k}})$ stencil only uses points of the $\mathbf{k} = (k_1)$ first rank is at most sixth order.*

Proof: For $\mathbf{k} = (k_1)$, $0 \leq n \leq d$ and $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 \geq \cdots \geq \lambda_n \geq 1$ we use the coefficients $(S_{\mathbf{k}}(m_{\boldsymbol{\lambda}}))_{\boldsymbol{\lambda},\mathbf{k}} = (2^{k_1}\binom{d-n}{k_1-n})_{n,k_1}$, which only depend on n and k_1. Table 1.2 provides the twelve conditions required to reach the 8th order:

$$\begin{aligned}
c^u_{\emptyset} &= 0 \\
c^u_{\mathbf{1}} &= 2c^v_{\emptyset} \neq 0 \\
c^u_{\mathbf{2}} &= 12c^v_{\mathbf{1}} && (2.28)\\
c^u_{\mathbf{11}} &= 4c^v_{\mathbf{1}} && (2.29)\\
c^u_{\mathbf{3}} &= 30c^v_{\mathbf{2}} \\
c^u_{\mathbf{21}} &= 2c^v_{\mathbf{2}} + 12c^v_{\mathbf{11}} \\
c^u_{\mathbf{111}} &= 6c^v_{\mathbf{11}} \\
c^u_{\mathbf{4}} &= 56c^v_{\mathbf{3}} && (2.30)\\
c^u_{\mathbf{31}} &= 2c^v_{\mathbf{3}} + 30c^v_{\mathbf{21}} && (2.31)\\
c^u_{\mathbf{22}} &= 24c^v_{\mathbf{21}} && (2.32)\\
c^u_{\mathbf{211}} &= 4c^v_{\mathbf{21}} + 12c^v_{\mathbf{111}} \\
c^u_{\mathbf{1111}} &= 8c^v_{\mathbf{111}}.
\end{aligned}$$

As $\mathbf{k} = (k_1)$, the lines $c^u_{\boldsymbol{\lambda}}$ only depend on n the number of non-zero λ_i (see Eq. (2.13)). Hence, we deduce $c^u_{\mathbf{1}} = c^u_{\mathbf{2}} = c^u_{\mathbf{3}} = c^u_{\mathbf{4}} \neq 0$, $c^u_{\mathbf{11}} = c^u_{\mathbf{21}} = c^u_{\mathbf{31}} = c^u_{\mathbf{22}}$ and $c^u_{\mathbf{111}} = c^u_{\mathbf{211}}$. For $d \geq 2$, Eqns. (2.28) and (2.29) imply that $c^u_{\mathbf{2}} = 3c^u_{\mathbf{11}}$ and Eqns. (2.30), (2.31) and (2.32) imply that $c^u_{\mathbf{31}} = \frac{1}{28}c^u_{\mathbf{4}} + \frac{5}{4}c^u_{\mathbf{22}}$. So taken together, it means that $c^u_{\mathbf{1}} = 0$ which is excluded. Hence, the sixth order limitation.

2.3 Useful properties of the compact schemes for applications

The method presented in this manuscript and providing Theorem 1.2 allows the conception of a large number of various compact finite difference schemes to solve the

Poisson equation. According to the context, some properties of these solvers are invaluable: the number m of activated ranks ($\mathbf{k} = (k_1, k_2 \ldots, k_m)$), the number of coefficients in A or B, the sign and distribution of the coefficients $a_{\mathbf{k}}$ (for the *Discrete Maximum Principle*, $a_{\mathbf{0}} < 0$ and $a_{\mathbf{k}} \geq 0$, $\forall \mathbf{k} \neq \mathbf{0}$) or the possibility of tensorizing the computation of $u \mapsto Au$.

2.3.1 Number of active points in A

The introduction of non-periodic boundary conditions may limit the number of activated ranks to one. Then, in a dimension of at least two, limiting $\mathbf{k}$ to (k_1) for A implies limiting the order of the solver to the sixth order whatever the dimensionality as proven in Section 2.2. Limiting both the A and B coefficients to the first rank restrains the maximal order to the fourth one, as we will see below in Eqn. (2.48). In the case of refinement domain boundaries, the number of activated ranks is not limited. Hence the interest of higher order compact schemes for the Adaptive Mesh Refinement framework.

To bound the number of elementary operations in the computer program, it can be interesting to minimize the number of active points in A. For each parameter $\mathbf{k}$, the number of elements of the symmetric group $\Sigma_{\mathbf{k}}$ is given by Lemma 1.1 : $S_{\mathbf{k}}(1) = 2^{\mathbf{k}}\binom{d}{\mathbf{k}}$.

2.3.2 Signs of the coefficients $a_{\mathbf{k}}$

Ideally, to apply the iterative Gauss-Seidel method to solve system (0.2) we need that the compact scheme satisfies the *Discrete Maximum Principle* and more precisely that $a_0 < 0$ be as small as possible and all the other $a_{\mathbf{k}}$ coefficients be ≥ 0 if $\mathbf{k} \neq 0$, in particular the a_1 coefficient related to the points next to $\mathbf{0}$ should be as large as possible. This optimizes the iterative algorithm relying on the matrix A to solve the linear system $Au = f = Bv$.

2.3.3 Distribution of the coefficients

To multiply by two the speed of convergence of the iterative multigrid method with Gauss-Seidel as smoothing, it suffices to update only a part of the values in u. For instance, in dimension two, we compute all the new iterates of u_{ij} for even values of $i+j$ and then for odd-numbered $i+j$ parameters. This is called red-black ordering [7]. To apply this technique efficiently, we need the condition $0 \leq a_{\mathbf{k}} \ll a_1$ for all even $\sum_i i * k_i$ to be satisfied ($a_{\mathbf{k}} = 0$ for all even $\sum_i i * k_i$ even conserves the symmetries of the numerical problem).

2.3.4 The possibility to compute $u \mapsto Au$, direction by direction

When the number of dimensions d increases, the $S_{\mathbf{k}}(1)$ number of points of $\Sigma_{\mathbf{k}}$ where $S_{\mathbf{k}}(1) = 2^{\mathbf{k}}\binom{d}{\mathbf{k}}$, rises dramatically. Summing so many points may be algorithmically and computationally exhausting. A way to simplify this step is to tensorize the operator A, direction by direction, at least partially. This allows the implementation

complexity and the computational time to be reduced. This will be presented in Part 2.6.

2.4 A two dimensional 18th order compact scheme for the Laplace equation

In [22], the author only considers points along the axes and the diagonals. It allows him to disclose a two dimensional 14th order compact scheme for the Laplace equation. Using a more general geometry we are able to obtain a 18th order compact scheme for the Laplace equation. We activate the two ranks of coefficients in the matrix A: a_0, a_1, a_2, a_{01}, a_{11} and a_{02}.

In addition to the four conditions (2.18), (2.19), (2.20) and (2.21) from Section 2.2, to reach the 14th order we must add a linear combination of rows **6**, **51**, **42** and **33** of the continuation of Table 1.2:

$$c^u_{\mathbf{6}} - 66\,c^u_{\mathbf{51}} + 495\,c^u_{\mathbf{42}} - 462\,c^u_{\mathbf{33}} = 0$$

which provides the condition:

$$a_1 - 64 * a_2 + 4096 * a_{01} + 23506 * a_{11} - 262144 * a_{02} = 0.$$

The last condition allowing the 18th order to be reached is given by a linear combination of rows **8**, **71**, **62**, **53** and **44**:

$$c^u_{\mathbf{8}} - 120\,c^u_{\mathbf{71}} + 10920\,c^u_{\mathbf{62}} - 48048\,c^u_{\mathbf{53}} - 38610\,c^u_{\mathbf{44}} = 0$$

which provides the condition:

$$a_1 + 2726 * a_2 + 65536 * a_{01} + 20988226 * a_{11} + 178651136 * a_{02} = 0.$$

We add the normalization of the coefficients by $\frac{1}{h^2} Au = \Delta u + o(h)$. It translates into:

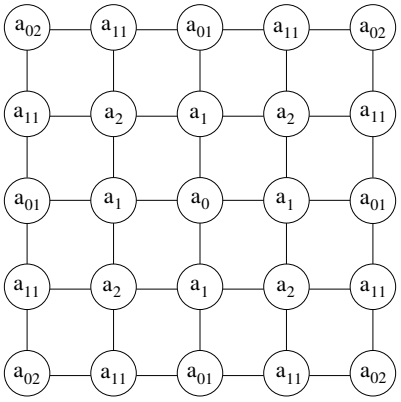
$$a_1 + 2 * a_2 + 4 * a_{01} + 10 * a_{11} + 8 * a_{02} = 1.$$

Then we obtain the coefficients:

$$a_0 = -\frac{2838953}{817278}, \quad a_1 = \frac{889264}{1225917}, \quad a_2 = \frac{549184}{3677751}, \tag{2.33}$$

$$a_{01} = -\frac{18881}{2451834}, \quad a_{11} = \frac{392}{525393}, \quad a_{02} = -\frac{233}{2674728}. \tag{2.34}$$

This stencil can be visualized as:



2.5 A three dimensional tenth order compact scheme for the Poisson equation

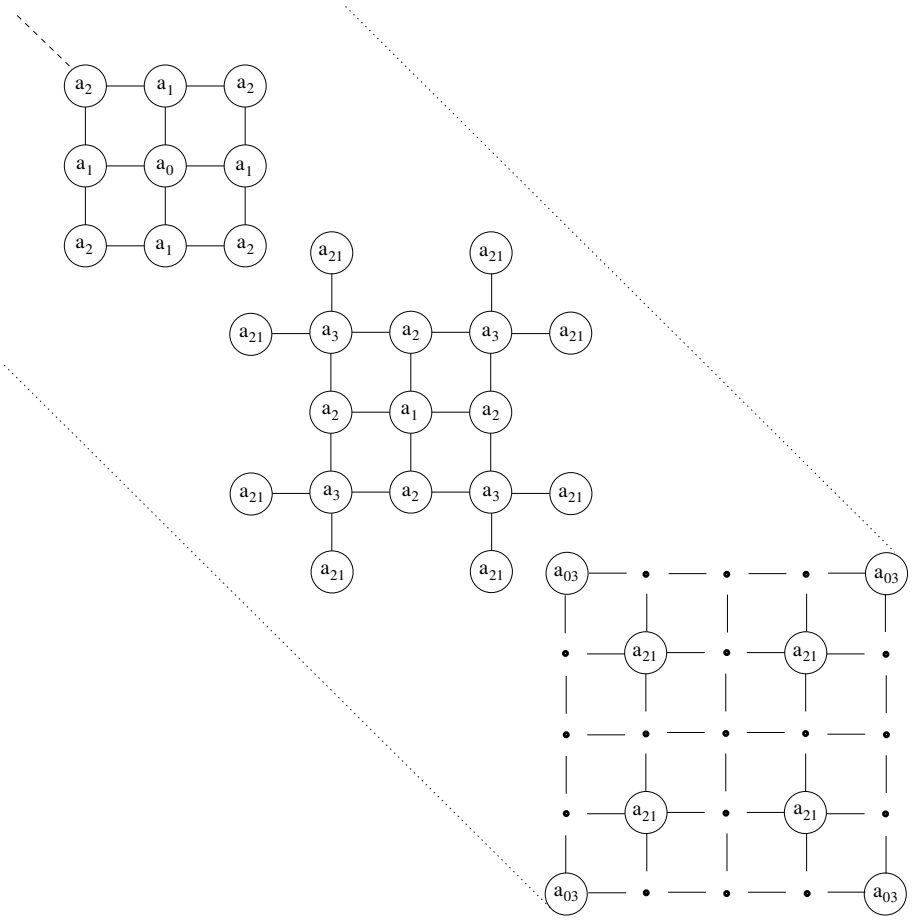
In dimension three we reach the tenth order when we activate the 59 points of the stencil corresponding to the coefficients a_0, a_1, a_2, a_3, a_{21} and a_{03}. Then, solving the five Eqns. (2.22)–(2.27), for A we find:

$$a_0 = -\frac{11755}{2814}, \quad a_1 = \frac{3152}{7035}, \quad a_2 = \frac{752}{7035}, \quad a_3 = \frac{29}{1407}, \tag{2.35}$$

$$a_{21} = \frac{4}{2345}, \quad a_{03} = \frac{1}{16080}. \tag{2.36}$$

These coefficients provide a matrix A that satisfies the *Discrete Maximum Principle*: a_0 is the only negative coefficient. Hence it is well-conditioned to apply the Gauss-Seidel method.

The bottom half of this symmetric three-dimensional stencil can be visualized as:



Moreover if we activate the 113 points of the stencil corresponding to the coefficients b_0, b_1, b_2, b_3, b_{01}, b_{11}, b_{02}, b_{03}, b_{001}, b_{101}, b_{0001} for B, then we find:

$$b_0 = \frac{10666253}{20260800}, \quad b_1 = \frac{130433}{2170800}, \quad b_2 = \frac{160117}{15195600}, \quad b_3 = \frac{182}{45225}, \tag{2.37}$$

$$b_{01} = -\frac{17021}{2701440}, \; b_{11} = -\frac{22}{37989}, \; b_{02} = -\frac{743}{243129600}, \; b_{03} = \frac{1013}{162086400}, \tag{2.38}$$

$$b_{001} = \frac{18883}{21273840}, \quad b_{101} = \frac{221}{4341600}, \quad b_{0001} = -\frac{10781}{141825600}. \tag{2.39}$$

2.6 Sixth order compact schemes in arbitrary dimensions

In this part of the manuscript, we will explicitly compute the coefficients of the operators A and B that form a sixth order compact finite difference scheme in Eq. (0.2) in an arbitrary dimension d. This generalizes the three-dimensional *HOC stencil*. Meanwhile we will show the necessity to activate the second rank of coefficients in B (or in A, but this is less interesting) to pass from the fourth order to the sixth. We will also give a partially tensorized solution, which presents numerous practical advantages.

We look for solutions A and B to problem (1.8) where the coefficients $(a_{\mathbf{k}})$ and $(b_{\mathbf{k}})$ apply to symmetric groups of points in Eq. (0.2). We only activate first rank coefficients for $a_{\mathbf{k}}$ i.e. a_k with $0 \leq k \leq d$ and we activate b_k for $0 \leq k \leq d$ as well as b_{01}.

Lemmas 1.1 and 1.2 allow an explicit computation of the coefficients $S_k(m_{\boldsymbol{\lambda}})$ for $0 \leq k \leq d$, $0 \leq n \leq d$ and $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_n) \in \mathbb{N}^{*n}$:

$$S_k(m_{\boldsymbol{\lambda}}) = S_k^n = 2^k \binom{d-n}{k-n}, \tag{2.40}$$

as well as $S_{01}(1) = 2d$, $S_{01}(\partial_1^2) = 8$, $S_{01}(\partial_1^4) = 32$ and $S_{01}(\partial_1^2 \partial_2^2) = 0$ for $\mathbf{k} = (k_1, k_2) = (0\ 1)$.

The first seven rows of Table 1.2 give the Eqns. (2.14), (2.15), (2.16) and (2.17), for which we have to add the term in b_{01} except for (2.14), then

$$\sum_{k=0}^{d} S_k^0 a_k = 0, \tag{2.41}$$

$$\sum_{k=1}^{d} S_k^1 a_k = 2 \sum_{k=0}^{d} S_k^0 b_k + 2 S_{01}^0 b_{01} = 2, \tag{2.42}$$

$$\sum_{k=1}^{d} S_k^1 a_k = 12 \sum_{k=1}^{d} S_k^1 b_k + 12 S_{01}(\partial_1^2) b_{01}, \tag{2.43}$$

$$\sum_{k=2}^{d} S_k^2 a_k = 4 \sum_{k=1}^{d} S_k^1 b_k + 4 S_{01}(\partial_1^2) b_{01} \tag{2.44}$$

for the fourth order; plus

$$\sum_{k=1}^{d} S_k^1 a_k = 30 \sum_{k=1}^{d} S_k^1 b_k + 30 S_{01}(\partial_1^4) b_{01}, \tag{2.45}$$

$$\sum_{k=2}^{d} S_k^2 a_k = 2 \sum_{k=1}^{d} S_k^1 b_k + 2 S_{01}(\partial_1^4) b_{01} + 12 \sum_{k=2}^{d} S_k^2 b_k + 12 S_{01}(\partial_1^2 \partial_2^2) b_{01}, \tag{2.46}$$

$$\sum_{k=3}^{d} S_k^3 a_k = 6 \sum_{k=2}^{d} S_k^2 b_k + 6 S_{01}(\partial_1^2 \partial_2^2) b_{01}, \tag{2.47}$$

for the sixth order.

If we carry out the combination $5\times(2.43)-2\times(2.45)$, we obtain directly the coefficient b_{01}:

$$b_{01} = -\frac{1}{240}. \tag{2.48}$$

As it is necessarily not zero, this shows that there is no sixth order symmetric strictly compact scheme for A and for B.

Considering Eqns. (2.41), (2.42) and performing the linear combinations $(2.43)-3\times(2.44)$ and $15\times(2.46)-30\times(2.47)-(2.45)$, we obtain the following equations on (a_k):

$$\begin{aligned}
\sum_{k=0}^{d} S_k^0 a_k &= 0, \\
\sum_{k=1}^{d} S_k^1 a_k &= 2, \\
\sum_{k=1}^{d} S_k^1 a_k &= 3 \sum_{k=2}^{d} S_k^2 a_k, \\
15 \sum_{k=2}^{d} S_k^2 a_k &= 30 \sum_{k=3}^{d} S_k^3 a_k + \sum_{k=1}^{d} S_k^1 a_k.
\end{aligned}$$

Solving this system and replacing S_k^n by their binomial expressions we obtain:

$$\sum_{k=0}^{d} 2^k \binom{d}{k} a_k = 0, \quad \sum_{k=1}^{d} 2^k \binom{d-1}{k-1} a_k = 2, \tag{2.49}$$

$$\sum_{k=2}^{d} 2^k \binom{d-2}{k-2} a_k = \frac{2}{3}, \quad \sum_{k=3}^{d} 2^k \binom{d-3}{k-3} a_k = \frac{4}{15}. \tag{2.50}$$

For $d \leq 9$ we minimize the number of points of the stencil in A by activating a_0, a_1, a_2 and a_d. This choice provides:

$$a_0 = \frac{3d^2 - 29d - 4}{15}, \quad a_1 = \frac{16 - 3d}{15}, \quad a_2 = \frac{1}{10}, \quad a_d = \frac{2^{2-d}}{15}. \tag{2.51}$$

We can see that for $d \geq 6$ the coefficient a_1 becomes negative, which hampers the application of the Gauss-Seidel method. For $d \geq 10$, a_0 is positive, which is even more problematic.

Regarding (b_k), we activate b_0, b_1 and b_2 in addition to b_{01}. Eqns. (2.47) then (2.44) and finally (2.42) provide:

$$b_0 = \frac{8d^2 - 77d + 360}{360}, \quad b_1 = \frac{11 - 2d}{90}, \quad b_2 = \frac{1}{90}, \quad b_{01} = -\frac{1}{240}. \tag{2.52}$$

As the number of points in the stencil increases considerably with the number of dimensions, we consider an operator A with a stencil of the form:

$$A = \alpha[p \;\; 1 \;\; p]^d + \begin{array}{ccc} & \gamma & \\ & | & \\ \gamma - & \beta & - \gamma \\ & | & \\ & \gamma & \end{array} \tag{2.53}$$

that means

$$a_0 = \alpha + \beta, \quad a_1 = \alpha\, p + \gamma, \quad \text{and} \quad a_k = \alpha\, p^k \quad \text{for} \quad k \geq 2.$$

Then Eqns. (2.49) and (2.50) provide

$$\sum_{k=0}^{d} 2^k \binom{d}{k} a_k = \alpha \sum_{k=0}^{d} \binom{d}{k} (2p)^k + 2d\gamma + \beta = \alpha(1+2p)^d + 2d\gamma + \beta = 0, \tag{2.54}$$

$$\sum_{k=1}^{d} 2^k \binom{d-1}{k-1} a_k = 2\alpha p \sum_{k=1}^{d} \binom{d-1}{k-1} (2p)^{k-1} + 2\gamma = 2\alpha p(1+2p)^{d-1} + 2\gamma = 2, \tag{2.55}$$

$$\sum_{k=2}^{d} 2^k \binom{d-2}{k-2} a_k = 4\alpha p^2 \sum_{k=2}^{d} \binom{d-2}{k-2} (2p)^{k-2} = 4\alpha p^2 (1+2p)^{d-2} = \frac{2}{3}, \tag{2.56}$$

$$\sum_{k=3}^{d} 2^k \binom{d-3}{k-3} a_k = 8\alpha p^3 \sum_{k=3}^{d} \binom{d-3}{k-3} (2p)^{k-3} = 8\alpha p^3 (1+2p)^{d-3} = \frac{4}{15}. \tag{2.57}$$

Dividing Eq. (2.57) by Eq. (2.56) we obtain $\frac{2p}{1+2p} = \frac{2}{5}$ so

$$p = \frac{1}{3}.$$

Reintroducing this quantity into Eq. (2.56) we obtain $\frac{4}{9}\alpha \left(1 + \frac{2}{3}\right)^{d-2} = \frac{2}{3}$ so

$$\alpha = \frac{3}{2}\left(\frac{3}{5}\right)^{d-2}, \quad a_k = \frac{3^{d-k-1}}{2 \cdot 5^{d-2}} \quad \text{for} \quad 2 \leq k \leq d.$$

Replacing p and α by their actual values in (2.55) we obtain γ:

$$\gamma = \frac{1}{6}.$$

This provides:

$$a_1 = \frac{1}{6} + \frac{1}{2}\left(\frac{3}{5}\right)^{d-2}.$$

Finally, Eq. (2.54) allows computation of β:

$$\beta = -\frac{25+2d}{6}.$$

This implies:

$$a_0 = \frac{3}{2}\left(\frac{3}{5}\right)^{d-2} - \frac{25+2d}{6}.$$

We verify that for $d = 3$ we recover the *HOC stencil*.

The number of operations for one iteration of the Gauss-Seidel method is $1 + 2d^2 + 2^d$ per point in the case of the smallest stencil (2.51), while it is $1 + 5d$ in the tensorized case (2.53). Even when we take into account the fact that we cannot use red-black ordering in this latest case, it remains more interesting as soon as $d \geq 4$. Moreover it is easier to implement and better conditioned.

To these (a_k) values we can associate $(b_{\mathbf{k}})$ from expressions (2.52) or we can look forward to a tensorized version of the form:

$$B = \omega[q \;\; 1 \;\; q]^d + \begin{array}{ccccccc} & & b_{01} & & & & \\ & & | & & & & \\ & & 0 & & & & \\ & & | & & & & \\ b_{01} & - & \lambda & - & 0 & - & b_{01} \\ & & | & & & & \\ & & 0 & & & & \\ & & | & & & & \\ & & b_{01} & & & & \end{array}$$

which corresponds to $b_0 = \lambda + \omega$ and $b_k = \omega q^k$ for $k \geq 1$.

Using what we have already computed including $b_{01} = -\frac{1}{240}$, we obtain the following conditions:

$$\sum_{k=0}^{d} 2^k \binom{d}{k} b_k = 1 + \frac{d}{120},$$

$$\sum_{k=1}^{d} 2^k \binom{d-1}{k-1} b_k = \frac{1}{5},$$

$$\sum_{k=2}^{d} 2^k \binom{d-2}{k-2} b_k = \frac{2}{45}.$$

We solve these equations as we did previously for (a_k). Then we find:

$$q = \frac{1}{7}, \quad \omega = \frac{9}{10}\left(\frac{7}{9}\right)^d \quad \text{and} \quad \lambda = \frac{1}{10} + \frac{d}{120}.$$

These correspond to

$$b_0 = \frac{1}{10} + \frac{d}{120} + \frac{9}{10}\left(\frac{7}{9}\right)^d, \quad b_k = \frac{9}{10}\left(\frac{7}{9}\right)^d \frac{1}{7^k} \quad \text{for } k \geq 1$$

$$\text{and} \quad b_{01} = -\frac{1}{240}.$$

For $d = 3$, this corresponds to the parameter $\beta = \frac{1}{810}$ in the *HOC Stencil*, see Sec. 2.1.2.

3 Numerical experiments

We test the schemes we obtained in Sections 2.5 and 2.6. First the tenth order scheme in dimension three compared to lesser order schemes, then the sixth order tensorized scheme in dimensions two, three, four, five and six. With the help of these compact schemes, we solve the equation $\Delta u = v$ on $[0,1]^d$ with periodic boundary conditions and with:

$$v(\mathbf{x}) = \prod_{i=1}^{d} \sin(2\pi x_i + 1).$$

We compare the numerical result to the exact solution:

$$u(\mathbf{x}) = -\frac{1}{4\pi^2 d} \prod_{i=1}^{d} \sin(2\pi x_i + 1).$$

Then we plot the error.

The convergence to the numerical solution of the compact scheme is performed by a Gauss-Seidel method associated with multigrid algorithms following [7] and [4]. The convergence rate of the Gauss-Seidel method remains close to 0.2 per iteration. At each iteration, the residual is divided by five. Hence we need approximately 20 iterations to converge up to the computer rounding error.

Note that the final destination of these compact schemes is to solve the Poisson equation with an adaptive grid as presented in [4]. Here we just test their claimed accuracy.

3.1 Testing the tenth order scheme in dimension three

To carry out this test, we use the code and algorithms developed in [4]. This code includes the implementation of an octree that is useful to test schemes requiring a multigrid method. Obtaining the 113 neighboring points of the stencil for B and the 59 neighboring points of the stencil for A requires care but it can be implemented without difficulty. To keep things simple, we used a basic test case without boundary conditions or mesh refinement. These extensions will be described separately in a forthcoming manuscript. Nevertheless, the principles to achieve them are already presented in [4] for the fourth order and two-dimensional case.

The tenth order accuracy is perfectly validated, as is shown in Fig. 3.1. Each time h is divided by two, the difference from the exact solution is divided by one thousand in infinity norm. It converges up to the computer rounding error. We also display the errors for other schemes of lesser order:

- the usual second order scheme with $a_0 = -6$, $a_1 = 1$ and $b_0 = 1$,

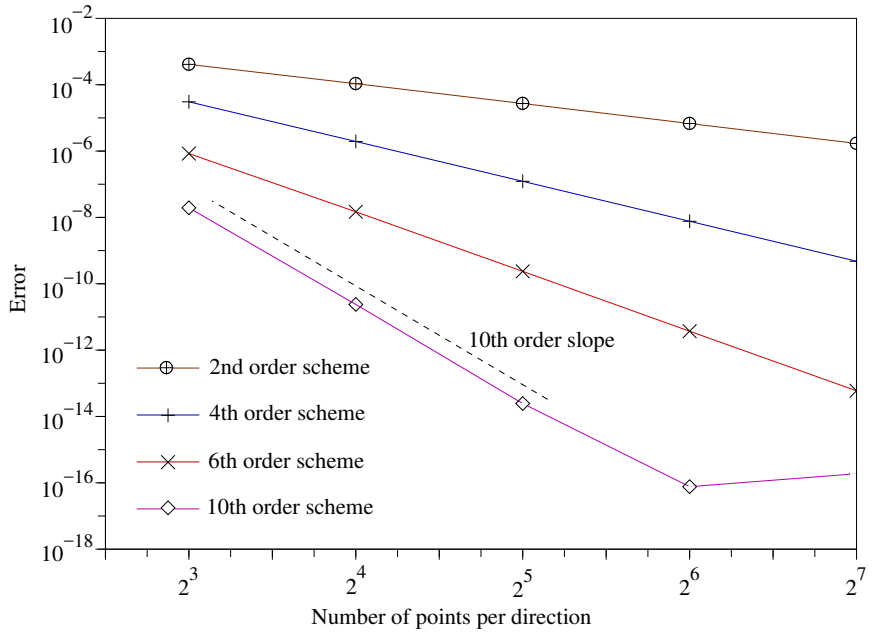


Fig. 3.1 Test of the tenth order scheme in dimension three presented in Section 2.5. Comparison with other schemes of lesser orders.

– a fourth order scheme extracted from [1] with

$$a_0 = -4, \quad a_1 = \frac{1}{3}, \quad a_2 = \frac{1}{6}, \quad b_0 = \frac{1}{2} \quad \text{and} \quad b_1 = \frac{1}{12},$$

– the sixth order *HOC Stencil* from Part 2.6 (the same as the one used in Fig. 3.2).

It shows the advantage of a higher order: the approximation reaches the exact solution up to machine rounding much faster.

3.2 Test of the tensorized sixth order scheme in an arbitrary dimension

The code from [4] allows any dimensional case from one to six to be treated. We have taken advantage of this to test the convergence of the tensorized scheme in Section 2.6, for which we expect a sixth order accuracy.

In Fig. 3.2 we demonstrate the expected order of accuracy except in the six-dimensional case for which there is a kind of hyperconvergence. Nevertheless, the small number of samples in this latest case prevents us from drawing any conclusions. When we switch to the slightly different condition

$$v(\mathbf{x}) = \sin(4\pi x_1 + 1) \prod_{i=2}^{d} \sin(2\pi x_i + 1),$$

we obtain the sixth order convergence for the six-dimensional case.

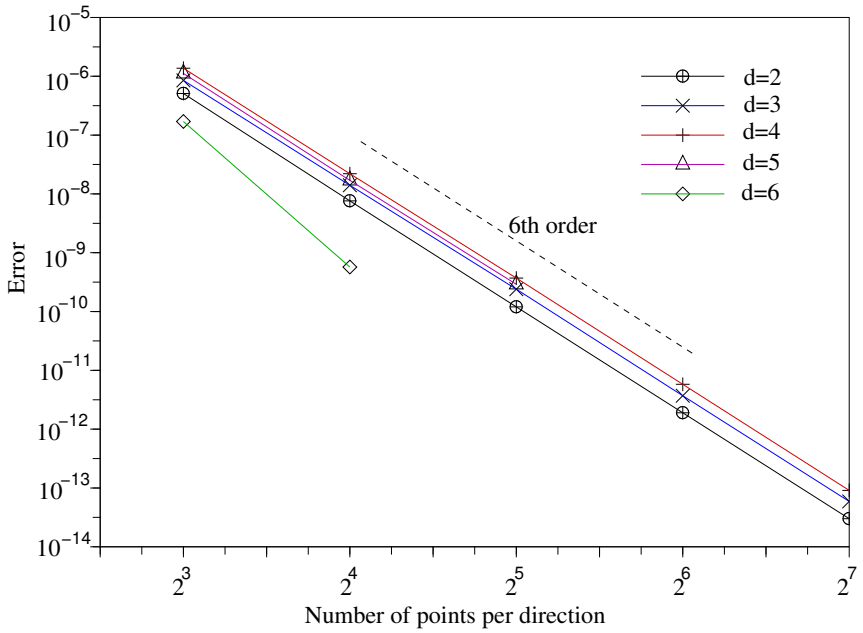


Fig. 3.2 Test of the sixth order scheme presented in Section 2.6 in various dimensions.

Conclusion

In this manuscript we have presented an original method using the symmetric polynomial algebra rather than Padé approximants [21] to compute the coefficients of compact finite difference schemes solving the Poisson equation. Meanwhile we have disclosed higher order schemes with relative ease. We have tested these conclusively in Section 3, which is dedicated to numerical experiments.

The increase in the order of accuracy for such a fundamental equation as the Poisson equation is of interest to many domains of Physics, such as magnetic reconnection [4] or *ab initio* chemistry [5]. In these domains the quality of the solutions depends crucially on the accuracy of the computations.

The joint use of high order schemes with AMR and multigrid techniques [23, 4] offers promising perspectives to solve problems in Physics which need high performance computing. Other perspectives include the application of the same kind of techniques to create original compact finite difference schemes for other operators than the Laplace operator (such as the Bilaplacian operator [3]), or for non Cartesian regular meshes [1,3] in arbitrary dimension. It is also possible to derive similar computations on irregular grids with minimal conditions on A in arbitrary dimension and to improve and generalize boundary stencils [10] for immersed boundary methods.

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