

Accepted Manuscript

A finite difference method with meshless interpolation for incompressible flows in non-graded tree-based grids

F.S. Sousa, C.F.A. Lages, J.L. Ansoni, A. Castelo, A. Simao

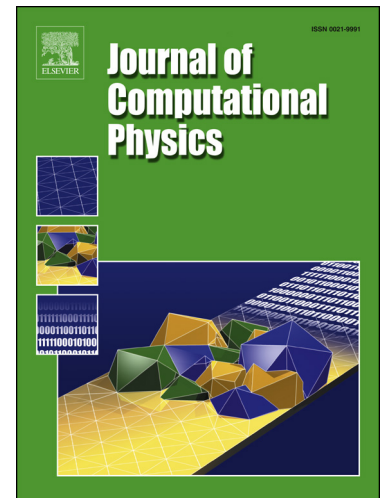
PII: S0021-9991(19)30496-6
DOI: <https://doi.org/10.1016/j.jcp.2019.07.011>
Reference: YJCPH 8812

To appear in: *Journal of Computational Physics*

Received date: 21 November 2018
Revised date: 3 July 2019
Accepted date: 4 July 2019

Please cite this article in press as: F.S. Sousa et al., A finite difference method with meshless interpolation for incompressible flows in non-graded tree-based grids, *J. Comput. Phys.* (2019), <https://doi.org/10.1016/j.jcp.2019.07.011>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Highlights

- A new finite difference method with meshless interpolations is presented
- Meshless interpolations are used to compute weights for the finite difference stencil
- Good alternative for geometric interpolations on non-graded quadtree/octree meshes
- 2D and 3D results show 2nd order convergence for both the solution and its gradient
- The method is extended for the Navier-Stokes model with good convergence results

1 A finite difference method with meshless interpolation
2 for incompressible flows in non-graded
3 tree-based grids

4 F. S. Sousa^{a,*}, C. F. A. Lages^a, J. L. Ansoni^a, A. Castelo^a, A. Simao^b

5 ^a*Department of Applied Mathematics and Statistics, Institute of Mathematical and
6 Computer Sciences, University of São Paulo at São Carlos, Brazil*

7 ^b*Department of Computer Systems, Institute of Mathematical and Computer Sciences,
8 University of São Paulo at São Carlos, Brazil*

9 **Abstract**

10 Tree-based mesh grids bring the advantage of using fast cartesian discretiza-
11 tions, such as finite differences, and the flexibility and accuracy of local mesh
12 refinement. The main challenge is how to adapt the discretization stencil near
13 the interfaces between grid elements of different sizes, which is usually solved
14 by local high-order geometrical interpolations. These interpolations depend on
15 the distribution of cells in the vicinity of the point of interest, hence they are
16 site-specific and can become quite complex in three-dimensional simulations,
17 specially when dealing with staggered unknown arrangements. Most meth-
18 ods usually avoid this by limiting the mesh configuration (usually to graded
19 quadtree/octree grids), reducing the number of cases to be treated locally. In
20 this work, we propose a robust method based on a moving least squares mesh-
21 less interpolation technique, which is employed to compute the weights of the
22 finite difference approximation in a given hierarchical grid, allowing for complex
23 mesh configurations, still keeping the overall order of accuracy of the resulting
24 method. Numerical convergence tests and application to fluid flow simulations
25 are performed to illustrate the flexibility, robustness and accuracy of this new
26 approach.

27 *Keywords:* Finite difference methods, Meshless interpolation, Moving least

28 squares, Tree-based grids, Navier-Stokes equations, Projection method

29 **1. Introduction**

30 The numerical solution of partial differential equations in general grids have
31 been sought by many researchers in last decades. Many schemes try to combine
32 efficiency and simplicity with the flexibility of unstructured mesh grids. A major
33 advantage is the ability to locally refine the mesh, improving the accuracy in
34 specific regions without drastically increasing the number of unknowns.

35 Among all possible ways of discretizing the spatial domain (simplicial meshes,
36 curvilinear meshes, chimera, and even meshless, among others), cartesian tree-
37 based hierarchical grids are a common choice. They allow for the development
38 of finite difference or finite volume methods, without the hassle of mapping and
39 transforming distorted elements or dealing with general and complicated sten-
40 cils, as happens in non-cartesian grids. Since fluxes are usually computed in
41 facets aligned with the cartesian axis, numerical schemes are usually simpler to
42 derive. Still, these facets are usually shared by different number of elements in
43 each side, which is the main difficulty for numerical methods for PDEs in such
44 grids. Different techniques to deal with this problem have been developed in
45 literature, most of them restricted to quadtree (in 2D) or octree (in 3D) meshes,
46 that are special cases of hierarchical grids represented by quadtree/octree data
47 structures. Despite this restriction, these tree-based data structures are gen-
48 eral enough and still a suitable choice for adaptive grids and moving fronts
49 [1, 2, 3, 4, 5, 6, 7].

50 Another type of hierarchical grids that share most of the difficulties above are
51 the block-structured meshes. They are composed of the superposition of patches
52 of structured grids of different resolutions, “glued” together by interpolation
53 schemes [8, 9, 10]. Such methods take advantage of the induced matrix structure

54 of the grid, not only demanding a careful mapping between all blocks, but also
55 adding a restriction on the adaptability of the mesh geometry.

56 Finite difference and finite volume methods in quadtree and octree meshes
57 for fluid flow simulations were first developed in late 1990's and early 2000's
58 ([1, 2, 11]). The main difficulty is to modify the FD/FV stencils near the
59 coarse/fine interfaces accordingly, which is usually performed by high-order in-
60 terpolations. Since these interpolations are mostly geometrical, they heavily
61 rely on the number of cells shared by each facet in the grid. Therefore, many of
62 these earlier schemes were developed in graded quadtree/octree meshes (see [2]),
63 which means that the characteristic mesh size reduction factor is restricted to
64 2:1 in coarse-to-fine interfaces. Thus, the number of possible configurations of
65 neighboring cells is reduced, allowing for hardcoding the interpolation formula
66 in each specific case. As well stated by Batty in [12], this restriction leads to an
67 unnecessary increase in the overall number of cells, motivating the recent de-
68 velopment of numerical methods for non-graded quadtree/octree meshes, such
69 as seen in [5, 13] for fluid flow simulations. However, while these numerical
70 approaches issue 2nd order convergence of the solved variables, their gradient
71 does not converge as such. Improved methods can be found in [12, 14], pre-
72 senting more sophisticated geometrical interpolations, however still only for the
73 numerical solution of Poisson equations.

74 Another way to overcome the limitations of geometrical interpolation is to
75 take advantage of meshless interpolations. Fully meshless methods are thor-
76 oughly available in the literature, however they still pose issues regarding con-
77 vergence and consistency, that are not completely solved (see for instance [15,
78 16, 17, 18, 19, 20, 21]). Conversely, much less references are found in hybrid
79 methods, that try to combine the simplicity of finite difference schemes with
80 meshless interpolations. Still, some remarkable work was developed in this di-

81 rection, mostly applied to the discretization of complex objects immersed in a
82 cartesian grid and in joining structured grids together (as seen in [22, 23, 24, 25]).

83 The present work brings a new development in the same direction. We em-
84 ploy meshless interpolations computed via moving least squares (MLS) in order
85 to modify finite difference stencils near the coarse-fine grid interfaces, as happens
86 in hierarchical meshes. The developed methodology is further investigated and
87 compared with non-graded octree-based methods, showing the advantages of
88 our new methodology in terms of accuracy and robustness, from simple Poisson
89 problems, to fluid flows in complex geometries.

90 **2. Finite difference approximation in hierarchical grids**

91 *2.1. Hierarchical grids (HiG)*

92 Our goal here is to present a general finite difference method that can be
93 applied to cartesian hierarchical grids represented by tree data structures. One
94 example of the generality of such hierarchical grid (HiG) can be seen in Fig. 1,
95 as well as the tree data structure representing it. In this data structure, each
96 leaf in the tree can be geometrically partitioned in any matrix arrangement of
97 cells. Particular cases are the quadtree in 2D and octree in 3D, in which this
98 division is restricted to four cells in 2D, and eight in 3D. Such general grids
99 impose difficulties for numerical schemes, specially those based on cartesian
100 finite difference (FD) approximations. They usually require the computation
101 of spacial interpolations in the unknown points of the FD stencil, that heavily
102 relies on the geometrical characteristics of the grid.

103 In order to avoid this geometrical dependence, we introduce a method based
104 on interpolations in a neighboring point cloud, requiring no geometry or topol-
105 ogy information, that is performed by an efficient MLS interpolation scheme.

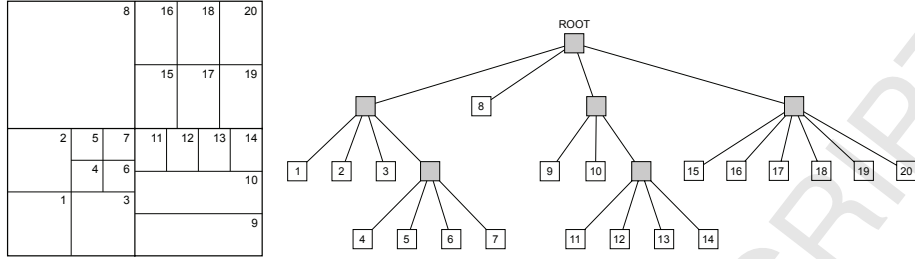
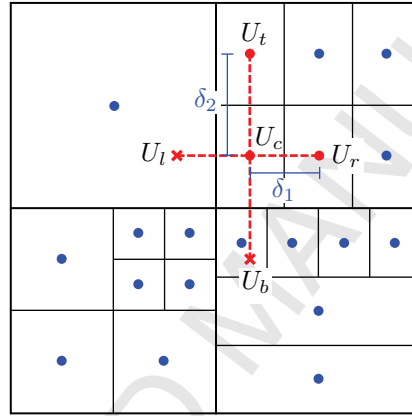


Figure 1: HiG tree data structure.

Figure 2: Finite difference 2nd order stencil discretization of a Poisson equation, where unknowns are located at cell centers. In this figure, δ_1 and δ_2 are the sizes of the cell containing the center point of the stencil.

106 2.2. Approximating derivatives in HiGs

107 To introduce the procedure to approximate derivatives with point cloud in-
 108 terpolation, suppose we need to solve a Poisson equation of the form

$$\nabla^2 u(x, y) = f(x, y) \quad (1)$$

109 in a rectangular domain $\Omega \in \mathbb{R}^2$ with suitable boundary conditions. Suppose
 110 we want to apply a standard 2nd order finite difference method to approxi-
 111 mate u at the centers of the cells defined in Fig. 2, resulting in the numerical

112 approximation

$$\frac{1}{\delta_1^2} (U_l - 2U_c + U_r) + \frac{1}{\delta_2^2} (U_t - 2U_c + U_b) = f_c, \quad (2)$$

113 where U_l, U_r, U_t, U_b, U_c are the approximation values of u at left, right, top,
 114 bottom and center position of the 5-point stencil, with sizes δ_1 in the x -direction
 115 and δ_2 in the y -direction. These sizes are defined as the corresponding sizes of
 116 the cell were the center point of the stencil lies. If the neighboring cells have
 117 the same size, the unknowns are aligned and no special treatment is required,
 118 resulting in the standard 5-point finite difference stencil. In a grid as general
 119 as the one in Fig. 2, we see that the approximation of u does not coincide
 120 with some of the mesh grid points (such as U_l and U_b), and those have to be
 121 approximated by some kind of interpolation of the grid unknowns in the vicinity
 122 of U_c . Such interpolation can be performed as

$$U_l = \sum_{k \in \mathcal{I}_l} w_k^l U_k \quad \text{and} \quad U_b = \sum_{k \in \mathcal{I}_b} w_k^b U_k \quad (3)$$

123 where $\mathcal{I}_l = \{i_k, k = 1, \dots, N_l\}$ and $\mathcal{I}_b = \{j_k, k = 1, \dots, N_b\}$ are the sets of
 124 indexes for the unknowns that are in the vicinity of U_c for each approximation.
 125 The coefficients w_k^l and w_k^b are computed by the interpolation procedure to be
 126 described later. The number of neighbors N_l and N_b depend on how many
 127 points are needed to keep the order of accuracy of the overall approximation. In
 128 a 2nd order approximation such as this, these interpolations should be at least
 129 3rd order accurate, which means that, in 2D, we will need at least 6 points to
 130 completely determine all coefficients of a 2nd degree interpolating polynomial,
 131 which will have a 3rd-order-accurate error. The final approximation will finally

132 read

$$\frac{1}{\delta_1^2} \left(\sum_{k \in \mathcal{I}_l} w_k^l U_k - 2U_c + U_r \right) + \frac{1}{\delta_2^2} \left(U_t - 2U_c + \sum_{k \in \mathcal{I}_b} w_k^b U_k \right) = f_c \quad (4)$$

133 or, in terms of the total number N_u of unknowns,

$$\sum_{k=1}^{N_u} A_{ck} U_k = f_c, \quad (5)$$

134 $c = 1, \dots, N_u$, that will result in a linear system of the form $\mathbf{A}\mathbf{u} = \mathbf{f}$ where each
135 line of A comes from approximations similar to Eq. (4).

136 This procedure is easily generalized for any finite difference stencil in hi-
137 erarchical meshes. The number of neighbors of U_c is computed based on the
138 expected order of accuracy. If there is not enough unknowns to keep the overall
139 order of the finite difference approximation (that can occur for example in coarse
140 grids), an adaptive stencil can be implemented, or a lower order interpolation
141 can be computed, for the sake of robustness. In the next section we show how
142 to efficiently compute the weights involved in the meshless interpolation.

143 *2.3. Discrete Moving Least Squares*

144 The procedure to complete the finite difference approximation in arbitrary
145 grids depends heavily on high order interpolations performed in the vicinity
146 of the unknown of interest. In our method, we perform these interpolations
147 by a Moving Least Squares (MLS) procedure. Although computation of MLS
148 basis functions is described in many works [15, 16, 18, 21], we introduce here an
149 efficient way of computing them for the high order interpolation needed by the
150 finite difference scheme.

151 Let us consider a set of n linearly independent smooth interpolation functions
152 $\Phi_i : \mathbb{R}^d \rightarrow \mathbb{R}$. Our goal is to interpolate the value of a function $u : \mathbb{R}^d \rightarrow \mathbb{R}$ such

153 that the approximation is given by

$$U(\mathbf{x}) = \sum_{j=1}^n c_j \Phi_j(\mathbf{x}) . \quad (6)$$

154 In our implementations, polynomial functions of several variables $\Phi_i(\mathbf{x}) = x_1^{\beta_1^i} \cdot$
 155 $x_2^{\beta_2^i} \cdots x_d^{\beta_d^i}$ are used, where $\beta_j^i \in \mathbb{N}$, $j = 1, \dots, d$, such that polynomials will be
 156 of maximum degree $K = \max \sum_{j=1}^d \beta_j^i$.

157 Given a set of m known points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m \in \mathbb{R}^d$, $m > n$, and m associated
 158 function values $u_1 = u(\mathbf{x}_1), u_2 = u(\mathbf{x}_2), \dots, u_m = u(\mathbf{x}_m)$, the procedure to
 159 interpolate u at \mathbf{x} using MLS is to minimize the error function

$$E(\mathbf{c}) = \|U - u\|_2^2 = \langle U - u, U - u \rangle_\lambda = \sum_{i=1}^m (U(\mathbf{x}_i) - u_i)^2 \lambda_i(\mathbf{x}) \quad (7)$$

160 that is a norm induced by a weighted inner product defined over the weight
 161 functions

$$\lambda_i(\mathbf{x}) = \frac{1}{\|\mathbf{x} - \mathbf{x}_i\|_2} \quad (8)$$

162 that depends on the position \mathbf{x} (explaining the term *moving* in MLS). Therefore,
 163 the minimizer $\mathbf{c} = (c_1, \dots, c_n)$ depends on the position \mathbf{x} as well. In practice, a
 164 threshold value $\varepsilon > 0$ is used to avoid the weight functions to become indefinite.
 165 Let us define matrices $W(\mathbf{x}) \in \mathbb{R}^{m \times m}$, which is the diagonal weight matrix,
 166 defined by $W_{ij}(\mathbf{x}) = \delta_{ij} \sqrt{\lambda_i(\mathbf{x})}$, and $P \in \mathbb{R}^{m \times n}$ the evaluation of the polynomial
 167 basis over the points \mathbf{x}_i , with components $P_{ij} = \Phi_j(\mathbf{x}_i)$. Furthermore, defining
 168 the vector $\mathbf{u} = (u_1, \dots, u_m)$, the error becomes

$$E(\mathbf{c}) = \|WPC - W\mathbf{u}\|_2^2 . \quad (9)$$

169 The solution that minimizes this error is then given by

$$\mathbf{c}(\mathbf{x}) = (WP)^\dagger W\mathbf{u} \quad (10)$$

170 where $(\cdot)^\dagger$ denotes the pseudo-inverse of Moore-Penrose of a matrix [26]. In
 171 fact, since matrix WP is non-square, we can perform its QR decomposition,
 172 resulting in

$$WP = Q \begin{bmatrix} R \\ 0 \end{bmatrix} = [Q_{\parallel} \quad Q_{\perp}] \begin{bmatrix} R \\ 0 \end{bmatrix}, \quad (11)$$

173 where $Q \in \mathbb{R}^{m \times m}$ is an orthogonal matrix, $Q_{\parallel} \in \mathbb{R}^{m \times n}$, $Q_{\perp} \in \mathbb{R}^{m \times (m-n)}$ are
 174 submatrices of Q , and $R \in \mathbb{R}^{n \times n}$ is an upper triangular matrix. The error in
 175 Eq. (9) is then rewritten as

$$E(\mathbf{c}) = \|R\mathbf{c} - Q_{\parallel}^t W\mathbf{u}\|_2^2 + \|Q_{\perp}^t W\mathbf{u}\|_2^2 \quad (12)$$

176 such that the solution is given by

$$\mathbf{c}(\mathbf{x}) = R^{-1} Q_{\parallel}^t W\mathbf{u}, \quad (13)$$

177 and the minimum error value is $E(\mathbf{c}) = \|Q_{\perp}^t W\mathbf{u}\|_2^2$.

178 This procedure however results in the coefficients $c_j(\mathbf{x})$ in the linear combi-
 179 nation of the polynomial basis functions $\Phi_j(\mathbf{x})$ in Eq. (6). Since we intend to
 180 couple these approximations to the finite difference approximations of deriva-
 181 tives, we should compute the interpolation coefficients w_i that form the linear
 182 combination of the values u_i . From Eqs. (6) and (13), we have

$$U(\mathbf{x}) = \mathbf{c}^t \Phi = \mathbf{u}^t \underbrace{WQ_{\parallel} R^{-t}}_{\mathbf{w}} \Phi = \sum_{i=1}^m w_i(\mathbf{x}) u(\mathbf{x}_i). \quad (14)$$

183 The approximation $U(\mathbf{x})$ should also interpolate $u_i = u(\mathbf{x}_i)$ at the points \mathbf{x}_i ,
 184 such that Eq. (6) yields

$$u_i = U(\mathbf{x}_i) = \sum_{j=1}^n c_j \Phi_j(\mathbf{x}_i), \quad (15)$$

185 and therefore

$$U(\mathbf{x}) = \sum_{i=1}^m w_i u(\mathbf{x}_i) = \sum_{i=1}^m w_i \sum_{j=1}^n c_j \Phi_j(\mathbf{x}_i) = \sum_{j=1}^n c_j \sum_{i=1}^m w_i \Phi_j(\mathbf{x}_i) \quad (16)$$

186 where the dependency of c_j and w_i on \mathbf{x} was dropped by the sake of notation.
 187 Comparing to the definition of $U(\mathbf{x})$ in Eq. (6) results

$$\sum_{j=1}^n c_j \Phi_j(\mathbf{x}) = \sum_{j=1}^n c_j \sum_{i=1}^m w_i \Phi_j(\mathbf{x}_i) \quad (17)$$

188 which is true for every \mathbf{c} that is a solution of the least squares problem in Eq.
 189 (9), allowing us to conclude that

$$\Phi_j(\mathbf{x}) = \sum_{i=1}^m w_i \Phi_j(\mathbf{x}_i). \quad (18)$$

190 The main consequence of Eq. (18) is that interpolation by the MLS preserve
 191 important properties such as the exact recovery of the basis functions. Par-
 192 ticularly, since Eq. (18) is true for constant polynomial basis functions (say,
 193 $\Phi_1(\mathbf{x}) = 1$), the weights w_i satisfy the partition of the unity property, i.e.,

$$\sum_{i=1}^m w_i = 1. \quad (19)$$

194

195 The coefficients w_i computed in that way are then used to assemble the finite
 196 difference approximation matrix A as in Eq. (5). The procedure to compute

197 the coefficients w_i is summarized in Algorithm 1. These values are then used in
 198 the discretization stencil when needed, like in the example of Eq. (4). Clearly,
 199 $w_i = w_i(\mathbf{x})$, which means that this algorithm should be executed for each ap-
 200 proximation of $U(\mathbf{x})$ needed. The most computational demanding procedures
 201 in this algorithm are the QR decomposition and the solution of a triangular sys-
 202 tem. They are however local and therefore can be easily computed in parallel,
 203 and since the problems are relatively small, they can take advantage of GPU
 204 architecture as well. As long as the mesh is static, this procedure is computed
 205 only once as a pre-processing step, and the interpolation weights can be cached.

Algorithm 1 Computation of coefficients w_i using MLS interpolation.

- 1: Given $\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{x} \in \mathbb{R}^d, \Phi_1, \dots, \Phi_n \in \mathcal{P}_K(\mathbb{R}^d), m > n$
 - 2: Compute $W = [\delta_{ij} \sqrt{\lambda_i(\mathbf{x})}]$, $P = [\Phi_j(\mathbf{x}_i)]$, $\lambda_i(\mathbf{x})$ given by Eq. (8)
 - 3: Perform the QR decomposition of matrix WP , resulting in R and Q_{\parallel}
 - 4: Compute $\Phi = (\Phi_1(\mathbf{x}), \dots, \Phi_n(\mathbf{x}))^t$
 - 5: Solve triangular system $R^t \mathbf{d} = \Phi \Rightarrow \mathbf{d} = R^{-t} \Phi$
 - 6: Compute $\mathbf{w} = WQ_{\parallel} \mathbf{d}$
-

206 **Remark 1.** If $U(\mathbf{x})$ is a complete polynomial of degree $K = \max \sum_{j=1}^d \beta_j^i$, i.e.,
 207 when it contains all monomials of degree s , for $s = 0, \dots, K$, then the coeffi-
 208 cients w_i will be invariant under rigid transformations (rotations, reflections and
 209 translations). The proof can be easily derived by induction on the polynomial
 210 degree K . This result can be further used to build a hash table for the cached
 211 interpolations, reducing even further the overall computing cost. This feature
 212 is even more efficient in graded quadtree/octree meshes, since there are just few
 213 different configurations to be considered. Additionally, since all basis functions
 214 are fully recovered by the MLS interpolation, PDEs with zero truncation errors
 215 are solved exactly, as in standard finite difference techniques.

216 **Remark 2.** The points $\mathbf{x}_1, \dots, \mathbf{x}_m$ are taken in a vicinity of point \mathbf{x} , that is
 217 defined as a circle centered in \mathbf{x} with a given interpolation radius. The number of

218 points inside this vicinity should be enough to at least recover the basis functions
 219 used in the interpolation. If this is not satisfied, the result is reflected as zeroes
 220 in the diagonal of matrix R (from QR decomposition in Eq. (11)), which turns
 221 out to be singular. In that case, this vicinity can be adaptively increased to
 222 overcome this drawback, adding robustness to the computed approximation. In
 223 our results, the initial radius is taken as $3 \times \max\{\delta_1, \dots, \delta_d\}$, where δ_i are the
 224 corresponding sizes of the cell containing \mathbf{x} , and every time we detect zeroes on
 225 the diagonal of R , the interpolation radius is increased by $\min\{\delta_1, \dots, \delta_d\}$.

226 **Remark 3.** It is clear that the matrices produced by such procedure are sparse,
 227 with sparsity depending on the size of the neighborhoods used in the MLS, and
 228 are not symmetric. Therefore iterative linear solvers such as the Generalized
 229 Minimum Residual Method (GMRES) or the Bi-Conjugate Gradient Method
 230 (Bi-CG) and its variants are good alternatives to solve the resulting linear sys-
 231 tems.

232 **Remark 4.** Although the weights w_i computed by the MLS procedure satisfy
 233 the partition of the unity property, there can be negative values, hence it is
 234 not possible to ensure the diagonal dominance of the resulting finite difference
 235 linear system. It is possible however to extend the degrees of freedom of the MLS
 236 problem over the kernel of $(WP)^t$ such that solutions with the restriction $w_i \geq 0$
 237 can be computed, ensuring the diagonal dominance of the resulting matrix.
 238 Our numerical experience with many different computations with this method
 239 indicates that this workaround is somewhat costly and completely unnecessary.

240 *2.4. Dirichlet and Neumann boundary conditions*

241 Dirichlet and Neumann type boundary conditions are handled much like
 242 standard techniques in finite difference context. Each finite difference stencil,
 243 when hitting the boundaries, end up in requiring points outside the computa-
 244 tional domain. In the case of Dirichlet-type boundary conditions, the known

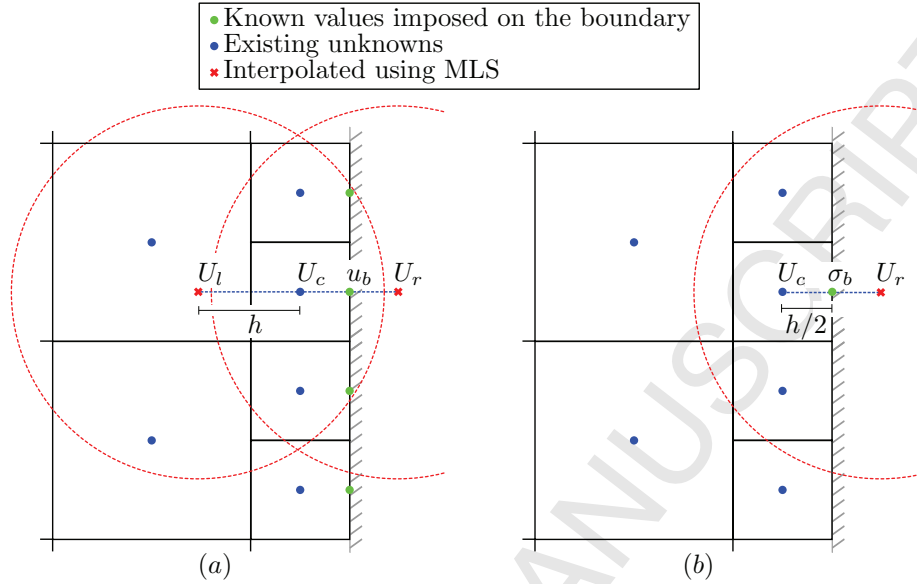


Figure 3: Discretization of the (a) Dirichlet and (b) Neumann boundary conditions using the meshless MLS interpolation.

245 values are added on the boundary, so that they are taken into account on every
 246 interpolation in the vicinity of the boundaries. An example is illustrated in
 247 Fig. 3(a), where the value u_b is imposed on all green dots (boundary values)
 248 such that the required MLS interpolations of U_l and U_r take those into account.
 249 This is very similar to standard finite difference techniques, where U_r would be
 250 computed such that the linear interpolation between U_c and U_r is exactly u_b .

251 In case of Neumann-type boundary conditions, say $\frac{\partial u}{\partial x} = \sigma_b$ on the right
 252 boundary, as depicted in Fig. 3(b), we discretize this boundary condition by
 253 standard finite differences, arriving at $U_r = U_c + h\sigma_b$, h being the size of the
 254 smaller cells near the boundary. Therefore, the stencil centered at U_c is modified
 255 accordingly. Variations of these two techniques are straightforwardly applied
 256 to different cell configurations and different unknowns positions with minor
 257 adaptations.

258 The interpolations are also affected by the lack of available points when

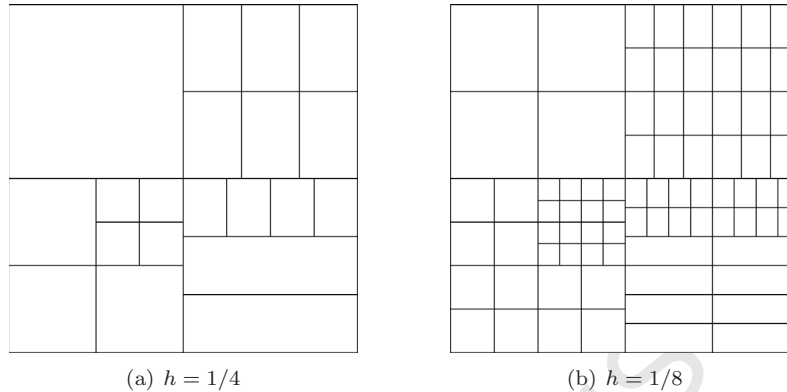


Figure 4: Two mesh refinements considered in the solution of the Poisson equation in a general HiG.

259 interpolating near boundaries, turning R singular and lowering the order of ap-
 260 proximation. In such cases, the interpolation radius is increased to complete
 261 the minimum requirements to keep the order of MLS interpolation. As seen in
 262 results later on, these simple techniques produce accurate and robust represen-
 263 tation of boundary conditions.

264 2.5. Verification: Poisson equation in a general HiG

265 In summary, the described method works as follows: whenever a finite dif-
 266 ference stencil is used to compute terms of the linear system matrix A , if the
 267 required point belonging to the stencil is available, it is used straight away. If
 268 it is missing, as occurring in the interface between different mesh sizes, MLS
 269 interpolations are used to compute the final weights entering matrix A .

270 To test this methodology and show the robustness of the method for a suffi-
 271 ciently general grid, we started with grid shown in Fig. 1 to discretize a square
 272 $\Omega = [-1, 1]^2$, which we attribute a reference mesh size of $h = 1/4$, the length of
 273 the smallest edge.

274 The described numerical method was then applied to this grid to solve a

Table 1: Errors and estimated order of convergence (EOC) for the Poisson equation in a general HiG.

h	$\ u - u_h\ _{L_2}$	EOC	$\ u - u_h\ _{L_\infty}$	EOC
1/4	1.29e-01	-	1.21e-01	-
1/8	7.06e-03	4.1	8.66e-03	3.8
1/16	1.30e-03	3.3	1.66e-03	3.1
1/32	2.32e-04	3.0	3.14e-04	2.9

275 Poisson equation (1) with analytical solution given by

$$u(x, y) = \sin(x) \cos(y) \quad (20)$$

276 with source term $f(x, y)$ and Dirichlet type boundary conditions manually com-
 277 puted as to result in this analytical solution. The MLS interpolations are per-
 278 formed with second degree polynomials. One can note that there are several
 279 interfaces with non-coincident cells (with the occurrence of many points, which
 280 are mostly known in finite element literature as “hanging nodes”). Refinement
 281 is carried out, subdividing uniformly each cell into four cells, to assess the nu-
 282 merical convergence for this case, with results reported in Table 1. The refined
 283 grids with reference sizes $h = 1/4$ and $h = 1/8$ are depicted in Fig. 4.

284 These results confirm the robustness of this method even when the mesh
 285 is divided in mostly non-coincident cells, with intensive use of interpolations
 286 all across interfaces. Evidently, this method can be further applied to connect
 287 domains discretized by different (non-coincident) meshes, however this type of
 288 application is not the main concern of the current work. We then move on to
 289 present more detailed results for non-graded quadtree/octree grids, in order to
 290 further extend this methodology to the solution of Navier-Stokes equations.

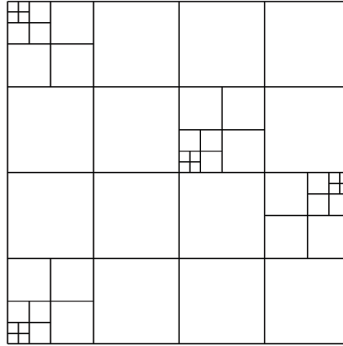


Figure 5: Non-graded mesh used in the Poisson convergence test.

291 *2.6. Verification: convergence in non-graded quadtree and octree meshes*

292 One of the main advantage of our methodology is the ability to preserve
 293 expected order of convergence without any special treatment or geometrical
 294 interpolations. This is specially advantageous when dealing with non-graded
 295 meshes, i.e., meshes that vary abruptly, with large cells being neighbors of very
 296 small ones. Any geometrical high-order interpolation would be site-specific, and
 297 difficult to program in higher dimensions.

298 To show that our method is capable of solving non-graded meshes, we per-
 299 formed tests by solving the Poisson equation (1) in non-graded quadtrees, as
 300 performed by other authors, such as Min et al. [14] and Batty [12]. The non-
 301 graded quadtree mesh is depicted in Fig. 5, discretizing a domain $[0, \pi]^2$ where
 302 (1) is solved with source term $f(x, y)$ computed as to yield an exact solution
 303 $u(x, y) = e^{-x-y}$, using Dirichlet-type boundary conditions. We computed nu-
 304 merical results for this problem using polynomial meshless interpolation de-
 305 scribed earlier, with polynomials of degree 2 and 3, that are reported in Tables
 306 2 and 3 respectively. The 2nd order accuracy is evident for u_h and ∇u_h when
 307 using 3rd degree polynomials, with a slight drop in the order of convergence for
 308 ∇u_h to around 1.6 when using 2nd degree polynomials.

309 To assess how the resulting linear systems are affected by our interpolation

Table 2: Errors and estimated order of convergence (EOC) for the numerical solution of the Poisson equation and its gradients, computed with 2nd degree interpolations in a non-graded quadtree with Dirichlet boundary conditions.

h	$\ u - u_h\ _{L_\infty}$	EOC	$\ \nabla u - \nabla u_h\ _{L_\infty}$	EOC
$\pi/32$	2.68e-2	-	2.57e-2	-
$\pi/64$	6.08e-3	2.1	1.07e-2	1.3
$\pi/128$	1.15e-3	2.3	3.18e-3	1.5
$\pi/256$	2.39e-4	2.3	1.03e-3	1.5
$\pi/512$	5.59e-5	2.2	3.24e-4	1.6
$\pi/1024$	1.43e-5	2.3	9.85e-5	1.6
$\pi/2048$	3.73e-6	2.1	3.03e-5	1.6
$\pi/4096$	8.72e-7	2.1	8.76e-6	1.6

Table 3: Errors and estimated order of convergence (EOC) for the numerical solution of the Poisson equation and its gradients, computed with 3rd degree interpolations in a non-graded quadtree with Dirichlet boundary conditions.

h	$\ u - u_h\ _{L_\infty}$	EOC	$\ \nabla u - \nabla u_h\ _{L_\infty}$	EOC
$\pi/32$	1.08e-2	-	7.01e-3	-
$\pi/64$	1.80e-3	2.6	2.36e-3	1.6
$\pi/128$	3.18e-4	2.5	6.96e-4	1.7
$\pi/256$	7.65e-5	2.4	1.70e-4	1.8
$\pi/512$	1.90e-5	2.3	4.40e-5	1.8
$\pi/1024$	5.19e-6	2.2	1.08e-5	1.9
$\pi/2048$	1.33e-6	2.2	2.81e-6	1.9
$\pi/4096$	3.36e-7	2.1	7.08e-7	1.9

Table 4: Observed condition numbers for the algebraic linear systems obtained with our method, for the Poisson convergence test using mesh from Figure 5.

h	Uniform grid estimate	Condition numbers from [12]	Observed condition numbers
$\pi/32$	4.205e+01	7.171e+01	1.116e+03
$\pi/64$	1.682e+02	2.815e+02	6.318e+03
$\pi/128$	6.728e+02	1.193e+03	3.297e+04
$\pi/256$	2.691e+03	4.713e+03	1.432e+05
$\pi/512$	1.076e+04	1.887e+04	5.960e+05
$\pi/1024$	4.306e+04	7.550e+04	2.419e+06
$\pi/2048$	1.722e+05	3.020e+05	9.754e+06
$\pi/4096$	6.889e+05	1.208e+06	3.921e+07

310 method, we compare the condition numbers of the linear system matrices to
 311 those observed in [12] for this exactly same problem, which can be seen in
 312 Table 4. Our condition numbers are consistently 32 times greater than those
 313 obtained by the geometric interpolation in [12], and roughly 55 times greater
 314 than a linear system obtained by a uniform mesh discretization with the same
 315 resolution as the finest grid cell in the corresponding non-graded quadtree mesh.
 316 This increase in the condition number is expected, since all the unknowns in the
 317 neighborhood of the MLS interpolation are connected, appearing as non-zero
 318 entries in the corresponding line of the final matrix. For this case, the condition
 319 number appears to be scaling with $\kappa(A) \approx 23/h^2$, as compared to the classical
 320 result for uniform grids $\kappa(A) \approx 4/(\pi^2 h^2)$, being both $\mathcal{O}(1/h^2)$. This difference
 321 however has little impact on the number of iterations required for convergence
 322 of iterative linear solvers.

323 One can also look at the fill-in effect on the matrix due to the MLS interpo-
 324 lations, which can be measured in terms of the number of non-zero entries for
 325 the matrices produced by our method as compared to a standard finite differ-
 326 ence discretization in uniform grids with the same number of unknowns. For
 327 the results reported in Table 3 using 3rd degree polynomials, the coarsest mesh
 328 $h = \pi/32$ yields a fill-in factor of about 6.2 times greater than the standard
 329 5-point stencil, while for $h = \pi/1024$ this factor drops to about 1.6, and for the
 330 finest grid with $h = \pi/4096$, the number of non-zeros in the MLS matrix is only
 331 about 1.2 times greater than a reference uniform finite difference discretization.

332 These results are similar to the ones found in [12], which employs a geomet-
 333 rical diagonal interpolation scheme, being difficult to extend in 3D. Our method
 334 is general and can easily be programmed for any number of spatial dimensions.
 335 To give an evidence of convergence in higher dimensions, we solved a 3D Pois-
 336 son problem in a cubical domain $[-\frac{\pi}{2}, \frac{\pi}{2}]^3$ with non-homogeneous Neumann

Table 5: Errors and estimated order of convergence (EOC) for the numerical solution of the 3D Poisson equation and its gradient, computed with 3rd degree interpolations in a non-graded octree with non-homogeneous Neumann boundary conditions.

h	$\ u - u_h\ _{L_\infty}$	EOC	$\ \nabla u - \nabla u_h\ _{L_\infty}$	EOC
$\pi/32$	2.14e-1	-	1.14e-1	-
$\pi/64$	5.22e-2	2.0	3.25e-2	1.8
$\pi/128$	1.23e-2	2.1	8.10e-3	2.0
$\pi/256$	2.12e-3	2.5	2.32e-3	1.8
$\pi/512$	4.62e-4	2.2	5.93e-4	2.0

337 boundary conditions, i.e.,

$$\nabla^2 u = f, \quad \mathbf{\hat{n}} \cdot \nabla u = g, \quad (21)$$

338 where functions $f = f(x, y, z)$ and $g = g(x, y, z)$ are prescribed so that the
339 manufactured exact solution for this problem is

$$u(x, y, z) = \cos(x) \cos(y) \cos(z). \quad (22)$$

340 The convergence test is performed using the same non-graded mesh found in
341 [4], originally employed for a Navier-Stokes problem. This initial mesh is de-
342 picted in Fig. 6 in which we associate a mesh size of $h = \pi/32$, the size of the
343 shortest edge. Results are shown in Table 5, where one can observe a 2nd order
344 convergence for both solution and its gradient.

345 The results presented in this section demonstrates the robustness and accu-
346 racy of our method for 2D and 3D Poisson problems with both Dirichlet and
347 Neumann boundary conditions, in non-graded quadtree and octree meshes. Al-
348 though not shown here, the extension of this method for even higher dimension
349 Poisson problems is straightforward, with similar results. In the next sections,
350 we extend this method for the incompressible Navier-Stokes equations using
351 standard projection methods, followed by verification and convergence results.

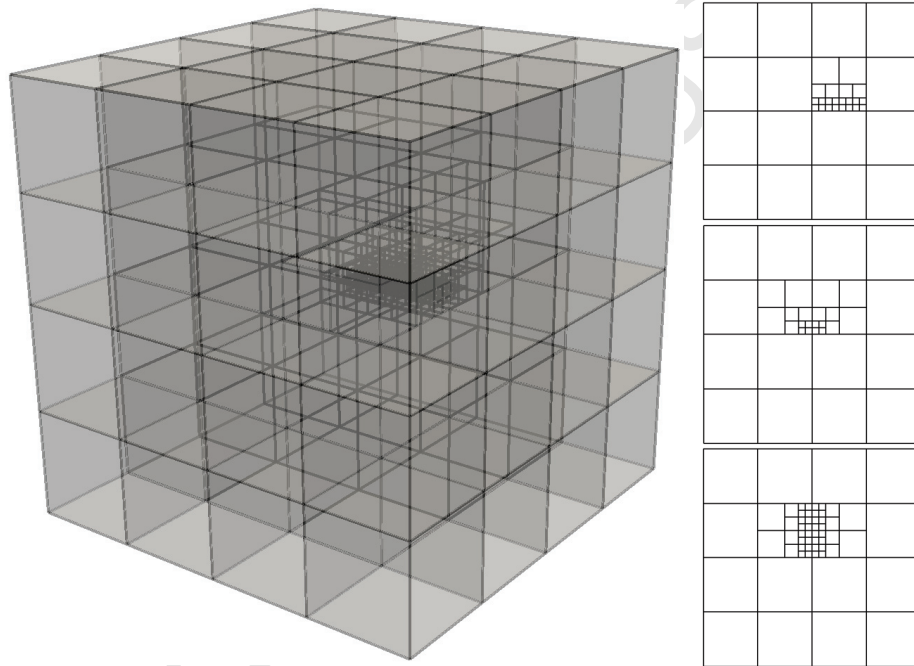


Figure 6: Non-graded mesh used for the 3D convergence test case, same as in [4]. On the left a 3D view of the mesh, and on the right three cut-planes corresponding to $x = 0$, $y = 0$ and $z = 0$ respectively, from top to bottom. They are oriented such that positive axis point always to the right and upwards.

352 **3. Discretization of the Navier-Stokes equations**

We are interested in the simulation of incompressible fluid flows using general hierarchical tree-based meshes, through our general meshless interpolation scheme, as discussed in last section. We begin with the well known model, the Navier-Stokes equations for newtonian fluid and incompressible flow, that in non-dimensional form reads

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u} + \mathbf{f} \quad (23)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (24)$$

353 where $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ denotes the velocity field and $p = p(\mathbf{x}, t)$ the pressure, both
 354 defined in a d -dimensional domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. The flow depends on the
 355 source term $\mathbf{f} = \mathbf{f}(\mathbf{x}, t)$ that could be used to model gravity or any other body
 356 force, and on the parameter Re , known as *Reynolds number*, that represents
 357 the ratio between inertial and viscous forces acting on the flow. Usually, $Re =$
 358 $U_\infty L / \nu$, with U_∞ and L being characteristic velocity and length, and $\nu = \mu / \rho$
 359 the kinematic viscosity, ratio between dynamic viscosity and density.

360 Many methods were developed since late 60's, resulting and many differ-
 361 ent approaches to deal with the strong coupling between velocity and pres-
 362 sure in the incompressible Navier-Stokes equations. A large number of such
 363 works implement the so called *Projection Method* or *Fractional Step Method*
 364 [27, 28, 29, 30, 31], which employs the well-known *Helmholtz-Hodge* decomposi-
 365 tion to split the Navier-Stokes operator allowing the sequential computation of
 366 velocity and pressure.

367 *3.1. Staggered grid arrangement*

368 As performed in many different works, we employ a staggered grid arrange-
 369 ment of the unknowns, which yields a stable discretization for uniform grids.

386 *3.2. The Helmholtz-Hodge decomposition*

387 The Helmholtz-Hodge decomposition theorem states that any vector field \mathbf{f}
 388 such that $\int_{\partial\Omega} \mathbf{f} \cdot \mathbf{n} = 0$ can be decomposed as a sum of a divergence-free vector
 389 field \mathbf{u} and a curl-free vector field \mathbf{v} , i.e., $\mathbf{f} = \mathbf{u} + \mathbf{v}$. Since \mathbf{v} is curl-free, there
 390 exists a scalar function p in such a way that $\mathbf{v} = \nabla p$, yielding the famous form

$$\mathbf{f} = \mathbf{u} + \nabla p \quad (25)$$

391 with $\nabla \cdot \mathbf{u} = 0$ and the normal components of \mathbf{f} and \mathbf{u} coinciding at the boundary
 392 of Ω .

393 This decomposition is often used to design numerical methods to solve the
 394 Navier-Stokes equations by means of segregating the coupled system of equa-
 395 tions, creating a sequential and therefore more efficient way to compute velocity
 396 and pressure. This is well known in the literature, and it is referred by as many
 397 names as there are variations. The most common terminology is “projection
 398 methods”, referring to the projection induced by the Helmholtz-Hodge decom-
 399 position theorem, of one vector field into the direct sum of divergence-free and
 400 curl-free spaces (other terminologies are known as Chorin’s method, MAC-type
 401 methods, fractional step methods, among others).

402 One of the main issues when employing the projection method in graded
 403 and non-graded tree-based meshes is the stability of the projection method by
 404 itself. For grids represented by quad/octrees, a sketch of a proof of stability,
 405 showing that the projection step does not introduce any spurious kinetic energy
 406 into the flow by itself, is shown in [5]. It relies on showing that there exist
 407 metrics (matrices) L_F and L_C such that the mimetic finite difference operators
 408 G and D satisfy the identity $L_F G = -(L_C D)^t$, which is further used to show
 409 that $\|\mathbf{u}^{n+1}\|_{L_F} \leq \|\mathbf{u}^*\|_{L_F}$, concluding the stability of the projection method.
 410 Although there is a small error in their definition of the metrics L_F and L_C

411 by assuming they are diagonal, which is not the case, the rest of the proof is
 412 correct (see [5]). Numerical observations support their theoretical result.

413 In a recent development, Olshanskii and co-workers [13] found that their dis-
 414 cretization, which is based on the work of Lossasso et al. [2], presents numerical
 415 instabilities in the computation of the discrete Helmholtz-Hodge decomposition
 416 in a staggered arrangement. They end up creating and implementing an arti-
 417 ficial filter to avoid those instabilities coming from their discretization (more
 418 details in [13]). More recently, Batty [12] presented numerical evidence of sta-
 419 bility of its central scheme with diagonal interpolations by successively applying
 420 the Helmholtz-Hodge decomposition.

421 Since our work intends to discretize the Navier-Stokes equations in general
 422 tree-based grids, we are motivated to perform the same tests as in [4, 5, 12, 13]
 423 to evaluate the stability of our discretization method.

424 The tests are based on the decomposition of a known vector field \mathbf{f} as in Eq.
 425 (25), by computing \mathbf{u} and p . To achieve this, we have to first solve the Poisson
 426 equation

$$\nabla \cdot \nabla p = \nabla \cdot \mathbf{f} , \quad \nabla p \cdot \mathbf{n}|_{\partial\Omega} = 0 \quad (26)$$

to find p , and finally compute \mathbf{u} from $\mathbf{u} = \mathbf{f} - \nabla p$. The test is performed in
 a square domain $\Omega = [0, 1]^2 \subset \mathbb{R}^2$, discretized by a two-level refinement mesh,
 where the characteristic mesh size is set to $h = h_{\min}$ for $x > \frac{1}{2}$ and $h = 2h_{\min}$
 for $x < \frac{1}{2}$, configuring the same setup as in [13]. In their work, they provide
 analytical expressions for \mathbf{u} and p that are used to compute known field \mathbf{f} and

$\nabla \cdot \mathbf{f}$, that are

$$\begin{aligned} u(x, y) &= \sin\left(\frac{2\pi(e^{ay} - 1)}{e^a - 1}\right) \left[1 - \cos\left(\frac{2\pi(e^x - 1)}{e - 1}\right)\right] \frac{ae^{ay}}{2\pi(e^a - 1)} \\ v(x, y) &= -\sin\left(\frac{2\pi(e^x - 1)}{e - 1}\right) \left[1 - \cos\left(\frac{2\pi(e^{ay} - 1)}{e^a - 1}\right)\right] \frac{e^x}{2\pi(e - 1)} \\ p(x, y) &= a \cos\left(\frac{2\pi(e^x - 1)}{e - 1}\right) \cos\left(\frac{2\pi(e^{ay} - 1)}{e^a - 1}\right) \frac{e^{a+1}}{(e - 1)(e^a - 1)} \end{aligned} \quad (27)$$

427 where $\mathbf{u} = (u, v)^t$ and $a = 0.1$.

428 Discretizations of the Poisson equation (26) are performed in a staggered
429 grid (p located at cell centers and normal components of \mathbf{u} and \mathbf{f} at cell facets,
430 as described earlier). A standard 2nd order 5-point finite difference stencil is
431 employed, with meshless interpolations using 2nd degree polynomials whenever
432 needed. We present a comparison of our results with those published in [13],
433 which are displayed in Figs. 8 and 9, in terms of the L_∞ and L_2 error norms
434 for \mathbf{u} and p , respectively. One can see that our method yields clean 2nd order
435 convergence for all error norms considered. Despite the fact that L_∞ error norm
436 for p is not shown in [13], we also computed errors with this norm to verify 2nd
437 order convergence as well. One can clearly see that Olshanskii's method and
438 both its variants Pressure Enrichment (PE) and Differential Filter (DF) did not
439 perform well, at least for the reported results from [13]. Results display only
440 first order convergence for the \mathbf{u} error in L_∞ norm, and less-than-second order
441 for the L_2 norm.

442 These results demonstrate the superiority of our method as compared to [13],
443 specially in terms of stability of the calculations around the interfaces between
444 cell refinements, even after the fixes proposed by the author.

445 The error for the x -component of the velocity vector can be seen in Fig. 10,
446 where small oscillations can be detected in our method, coming from the unbal-
447 ancing between fluxes across the coarse-to-fine interface. However they are no

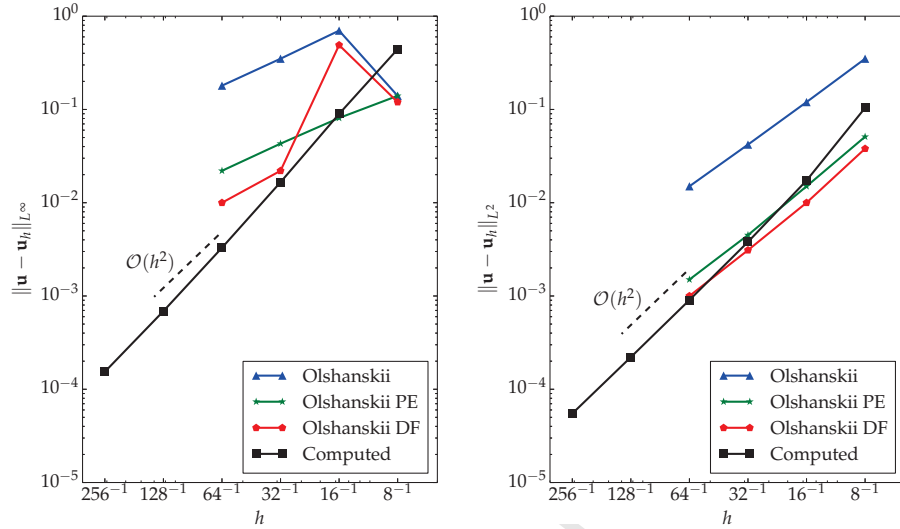


Figure 8: Error norms for the computed velocity field, as compared to Olshanskii's method and its variants.

448 bigger than the error elsewhere, and they do not increase (in fact they decrease)
 449 as the mesh is refined, which is a clear sign of stability for our discretization
 450 method.

451 Another numerical test for the stability of the projection via Helmholtz-
 452 Hodge decomposition can be found in the work of Min and Gibou [4], later
 453 reproduced by Guittet et al. [5] and more recently by Batty [12]. It comprises
 454 successive applications of the Helmholtz-Hodge decomposition, beginning with
 455 the initial vector field

$$\mathbf{u}^{(0)}(x, y) = \begin{bmatrix} \sin(x) \cos(y) + x(\pi - x)y^2 \left(\frac{y}{3} - \frac{\pi}{2}\right) \\ -\cos(x) \sin(y) + y(\pi - y)x^2 \left(\frac{x}{3} - \frac{\pi}{2}\right) \end{bmatrix}, \quad (28)$$

defined in $\Omega = [0, \pi]^2$, which is discretized by a non-graded mesh illustrated in Fig. 11. The procedure consists of solving a sequence of projections of the form

$$\mathbf{u}^{(k)} = \mathbf{u}^{(k+1)} + \nabla p^{(k+1)} \quad (29)$$

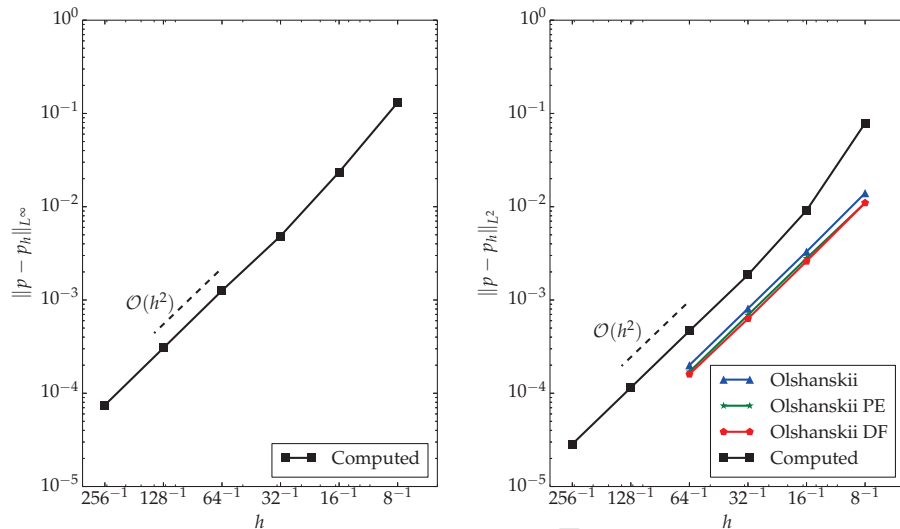


Figure 9: Error norms for the computed pressure, as compared to Olshanskii's method and its variants. Olshanskii et. al do not report pressure convergence in L_∞ norm.

456 where $\nabla \cdot \mathbf{u}^{(k+1)} = 0$, for $k \geq 0$. If the decomposition is stable, the error should
 457 stay stationary even over dozens of successive projections. Results are reported
 458 in Fig. 12, where one can see the log of the error $\|\mathbf{u}^{(k+1)} - \mathbf{u}^{(k)}\|_{L_\infty}$, which stays
 459 the same for as far as one hundred iterations, the same behavior as the results
 460 presented in [12] and [4].

461 3.3. Projection method for the Navier-Stokes equations

462 With the stability of the Helmholtz-Hodge decomposition verified, we move
 463 on to the discretization of the Navier-Stokes equations. We will briefly describe
 464 here the projection method used in the Navier-Stokes discretization, known
 465 as *incremental projection method* or *pressure correction method* (the reader is
 466 referred to throughout discussions about different types of projection methods
 467 in [28, 29, 31, 32, 33] and references therein).

468 Upon discretizing Eq. (23) in time using, for instance, a first order semi-
 469 implicit discretization, the idea of the incremental projection method is to use
 470 the pressure at the previous time step, which yields an implicitly-computed

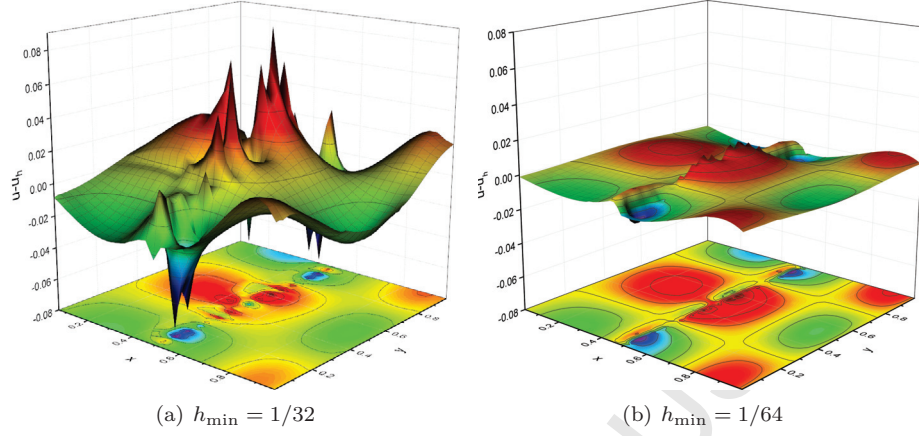


Figure 10: Error for the x -component of the velocity field for two different meshes, $h_{\min} = 1/32$ and $h_{\min} = 1/64$, illustrating how it behaves on refining.

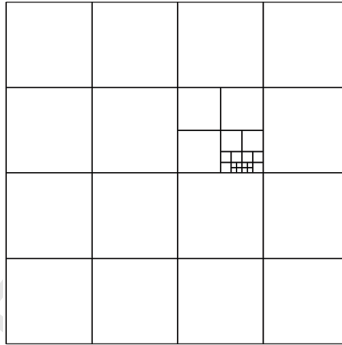


Figure 11: Non-graded mesh used in the projection stability test case.

471 velocity field \mathbf{u}^* that is not divergence free, by the solution of

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\delta t} = -\nabla p^n - \mathbf{u}^n \cdot \nabla \mathbf{u}^n + \frac{1}{Re} \nabla^2 \mathbf{u}^* + \mathbf{f}^n \quad (30)$$

472 with \mathbf{u}^* satisfying the same boundary conditions as \mathbf{u} . By applying the previ-
 473 ously discussed Helmholtz-Hodge decomposition to \mathbf{u}^* and defining the scalar
 474 $\varphi = -\delta t(p^{n+1} - p^n)$, the corrected velocity field can be computed from the

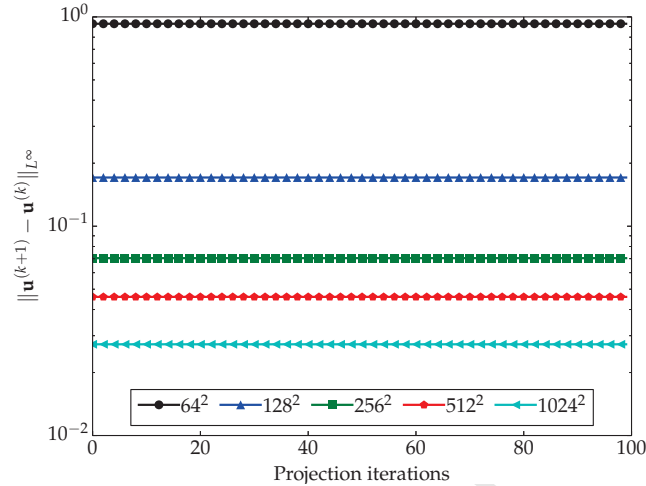


Figure 12: Log of the error $\|\mathbf{u}^{(k+1)} - \mathbf{u}^{(k)}\|_{L^\infty}$ after successive projections of the initial vector field.

475 decomposition itself (projection step) as

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \nabla\varphi \quad (31)$$

476 where φ is obtained by solving the Poisson problem

$$\nabla^2\varphi = \nabla \cdot \mathbf{u}^*, \quad (32)$$

477 obtained by computing the divergence of equation (31), with homogeneous Neu-
 478 mann boundary conditions $\mathbf{n} \cdot \nabla\varphi = 0$ on $\partial\Omega$. This procedure is computed
 479 sequentially (Eqs. (30) \rightarrow (32) \rightarrow (31)), therefore one time step of this method
 480 is much faster than computing one time step of the coupled problem, explaining
 481 its popularity. The incremental version of the projection method has a splitting
 482 error (unrelated to the time discretization) of the order of $\mathcal{O}(\delta t^2)$, allowing the
 483 choice of 2nd-order accurate methods for the time discretization.

484 The system in Eq. (30) is discretized in time by a semi-implicit scheme,
 485 where viscous part is implicit, but the convective part is kept at the previ-

486 ous time-step to linearize the system. As a consequence, the time step δt has
487 to satisfy the well known Courant-Friedrichs-Lewy (CFL) condition, which is
488 $\delta t \|\mathbf{u}\|_{\infty} / h_{\min} \leq 1$.

489 **Remark 5.** The non-incremental version of this projection method can be
490 achieved by setting $\nabla p^n = \mathbf{0}$ in the momentum equation. This is sometimes
491 referred as Chorin’s method [34], and has a $\mathcal{O}(\delta t)$ splitting error, hindering the
492 convergence of higher order time discretizations.

493 Spatial discretizations are performed for each step of the projection method
494 described above. A staggered arrangement of the unknowns is employed, as
495 explained in previous sections, avoiding known tensile instabilities. All dis-
496 cretizations are based on 2nd order accurate finite difference stencils, that are
497 used throughout the hierarchical mesh. As already addressed, the interface be-
498 tween different mesh sizes is handled by the newly developed MLS interpolation
499 technique.

500 In this work, for simplicity, we restrict ourselves to the case of low-Reynolds
501 numbers flows, therefore the non-linear (convective) terms of the Navier-Stokes
502 equations can be safely discretized by central differencing with MLS interpola-
503 tions for off-grid point assessments.

504 4. Numerical results

505 In this section we present numerical results for verification tests by solv-
506 ing the Navier-Stokes equations with manufactured solutions, both in 2D and
507 3D. We display the convergence curves for these academic problems compar-
508 ing to other results found in the literature. All simulations were performed
509 with the meshless interpolation scheme described in Section 2, coupled with
510 the projection method and time discretization both described in Section 3.3.
511 The resulting discrete linear systems are solved with the GMRES method, as

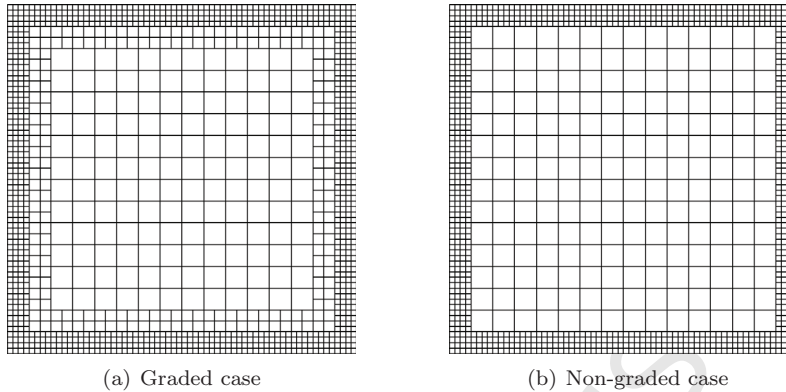


Figure 13: Meshes used in the 2D lid-driven cavity flow convergence test. Both correspond to $h_{\min} = 1/64$ and $h_{\max} = 1/16$

512 implemented in PETSc library [35, 36]. The last example in this section is a
 513 full three-dimensional simulation of a complex array of microchannels, using a
 514 locally-refined octree mesh, computed by our in-house parallel code that im-
 515 plements the techniques described in this work, illustrating the robustness and
 516 applicability of our methodology.

517 4.1. Lid-driven cavity flow in 2D

518 A simple 2D lid-driven cavity flow is simulated with the proposed method-
 519 ology. To assess the convergence rates for this case, we employed a test with
 520 manufactured analytical steady-state solution, published by Shih & Tan [37].
 521 As can be seen in [37], the manufactured solution for velocity and pressure
 522 consists of products of polynomials in x and y directions. The computational
 523 domain is set to be $\Omega = [0, 1]^2$, with $Re = 100$. We computed solutions for
 524 both graded and non-graded hierarchical meshes, starting with $h_{\min} = 1/64$
 525 and $h_{\max} = 1/16$, and the subsequent meshes are produced by divisions by two
 526 in each direction. The starting meshes used in this test can be seen in Fig. 13.

527 The simulations were performed solving the transient Navier-Stokes equa-
 528 tions for pseudo time-step marching until the steady-state solution is reached,

529 before computing the error norms. Figure 14 depicts the convergence of the
 530 L_2 -norm error for both velocity (left) and pressure (right), for both graded
 531 and non-graded meshes. Results are consistent with previous convergence tests,
 532 yielding clean 2nd order spatial convergence. Despite the fact that non-graded
 533 mesh has significantly less elements with sharper transitions between coarse and
 534 fine cells, the order of convergence is maintained, with slightly larger errors as
 535 expected, but still comparable to the graded case. This test was performed
 536 using 2nd order polynomial for the MLS interpolations.

537 4.2. Unsteady flow with analytical solution in 3D

538 We test the order of convergence for three-dimensional simulations in non-
 539 graded grids by reproducing the benchmark test found in [4], section 4.4. The
 540 domain is a cube $[-\frac{\pi}{2}, \frac{\pi}{2}]^3$ with $Re = 1$, for which the analytical solution can
 541 be found in [4]. We used the same grid as in their work, which is a non-graded
 542 octree, shown in Fig. 6 for the mesh size $h_{\min} = \pi/32$. The time step is chosen
 543 to be $\delta t = h_{\min}/4$, satisfying the CFL restriction. This value is however smaller
 544 than the time step in [4], since they use a semi-Lagrangian approach for the
 545 advective term, which is free from CFL-type restriction. As in their work we
 546 computed the numerical solutions up to a time $t = \pi$. Meshless interpolations
 547 are computed with 2nd degree polynomial basis, such as in the two-dimensional
 548 tests.

549 Results can be seen in Fig. 15, where the L_2 -norm of the error for the
 550 x -component of the velocity field is reported. The result computed with our
 551 method is compared to the results found in Min & Gibou [4], with close agree-
 552 ment between them. A slight advantage can be noticed for Min & Gibou's
 553 geometrical interpolation method for this case. Conversely, our method dis-
 554 plays a clean 2nd order convergence rate for all computed meshes. We also
 555 report pressure errors in Fig. 15 (right), but unfortunately, we could not find

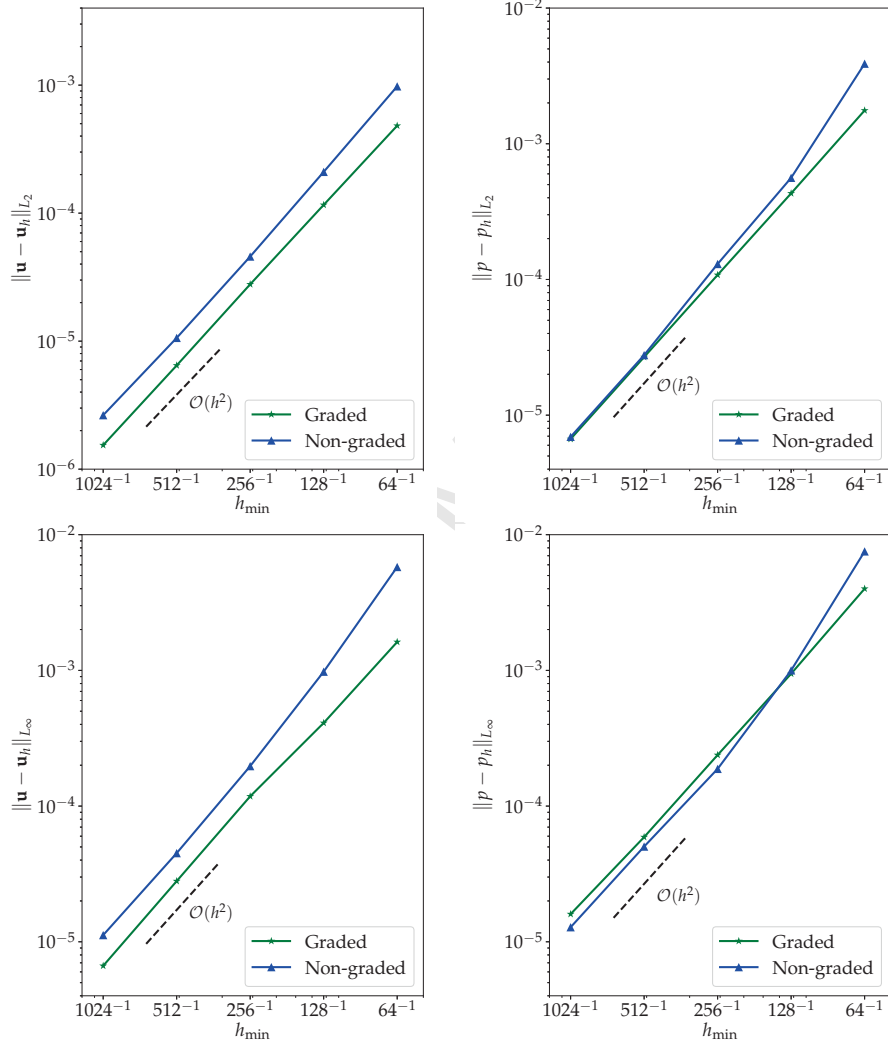


Figure 14: Convergence in the L_2 -norm (top) and L_∞ -norm (bottom) for both velocity (left) and pressure (right) errors, comparing graded and non-graded cases.

556 pressure errors in [4] for this test case to compare with our results. They do re-
 557 port however a convergence of $\mathcal{O}(h^2)$ for the divergence of the velocity field, that
 558 is not comparable to our method, since the discrete divergence of the solution is
 559 found to be constant circa 10^{-12} , independent of mesh size. This same behavior
 560 is observed in all Navier-Stokes simulations performed with our method.

561 4.3. Simulation of a complex 3D array of microchannels

562 In this test case, we simulate an incompressible single-fluid flow in an array
 563 of microchannels, introducing some level of geometric complexity in the three-
 564 dimensional flow domain. This test was designed specifically to demonstrate the
 565 simulation capabilities and robustness of the developed approximation method-
 566 ology, as well as the flexibility of the parallel in-house code implemented for this
 567 purpose, with aid of the PETSc library [35, 36].

568 The geometry, as well as boundary conditions, can be seen in Fig. 16.
 569 The total width, length and height are set to be respectively $W = 0.8 \text{ mm}$,
 570 $L = 2.4 \text{ mm}$ and $H = 0.4 \text{ mm}$. The inlet is a channel of $0.1 \text{ mm} \times 0.1 \text{ mm}$, where
 571 water at room temperature is injected with constant velocity of $U_{\text{in}} = 0.1 \text{ mm/s}$.
 572 Scaling this geometry by $\ell = 0.1 \text{ mm}$, and using $\nu \approx 10^{-6} \text{ m}^2/\text{s}$ as the kinematic
 573 viscosity of water at room temperature, we end up with a Reynolds number of
 574 $Re = \ell U_{\text{in}}/\nu = 10^{-2}$.

575 This array of microchannels is discretized by the union of several hierarchi-
 576 cal grids, with $h_{\text{min}} = \ell/40 = 2.5 \times 10^{-3} \text{ mm}$ and $h_{\text{max}} = \ell/10 = 10^{-2} \text{ mm}$,
 577 resulting a total of 1,517,704 elements, and approximately 6 million variables.
 578 Figure 17 shows slices of the 3D mesh to give an idea of the level of refine-
 579 ment used in each section of the mesh. The simulation was performed using
 580 $\delta t = 10^{-3} \text{ s}$ and the approximate solutions are computed until steady state is
 581 reached. Streamlines for this flow can be seen in Fig. 18. The result is qualita-
 582 tive, but demonstrates the robustness and applicability of this newly developed

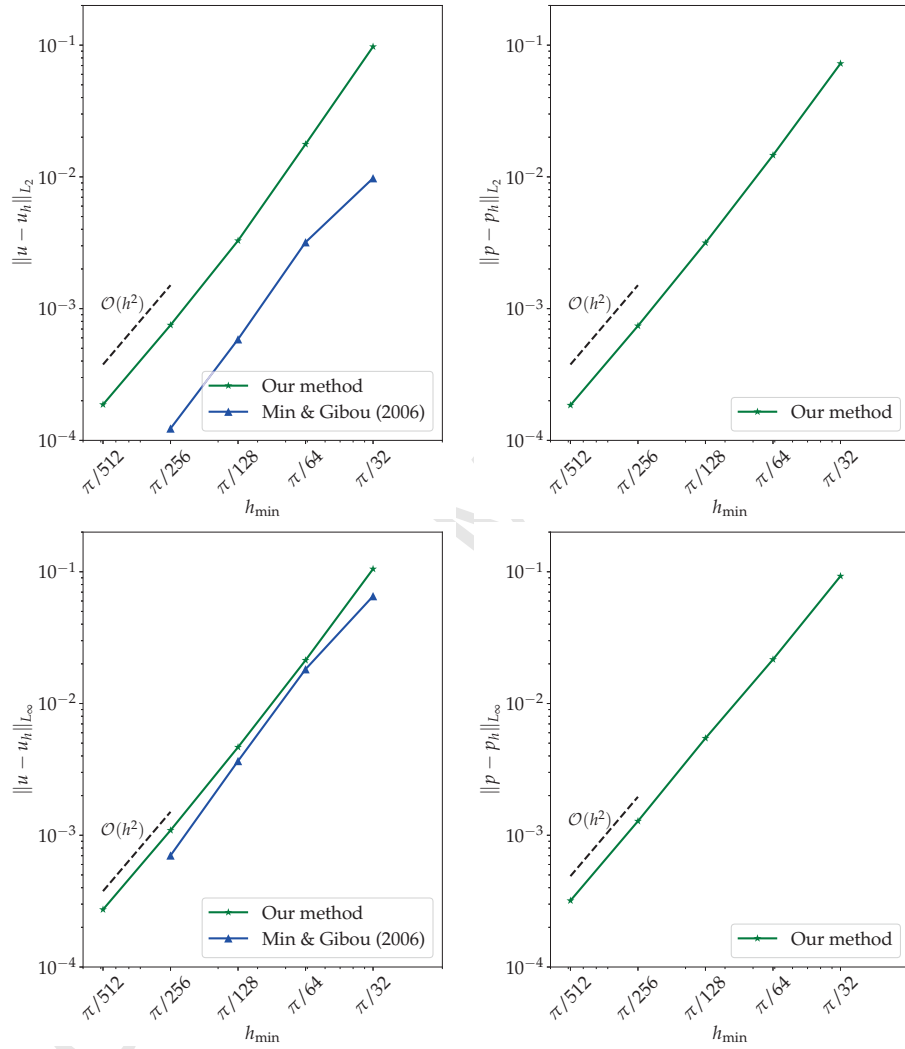


Figure 15: Convergence in the L_2 -norm (top) and L_∞ -norm (bottom) of the x -component of the velocity field (left) and pressure (right). Only the velocity error is compared to the results reported by Min et al. [4], since there is no information about pressure convergence in their work.

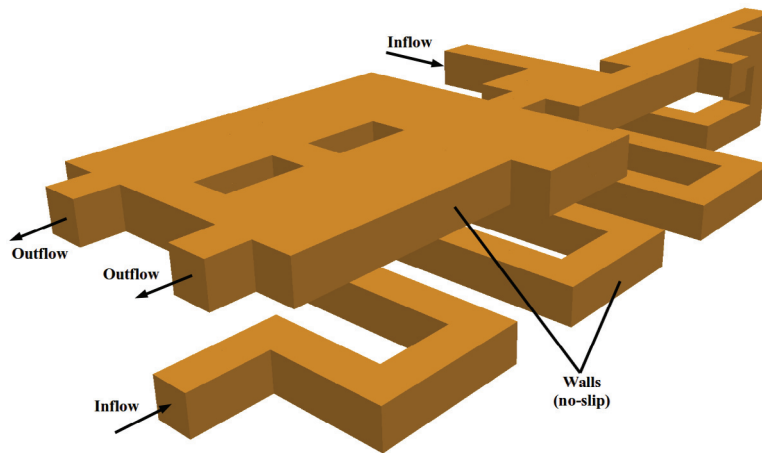


Figure 16: Microchannel problem configuration (Length $L = 2.4$, width $W = 0.8$ and height $H = 0.4$).

583 methodology.

584 5. Conclusions

585 A finite difference method with meshless interpolations in tree-based grids
 586 is presented. The method is capable of handling generic hierarchical tree-based
 587 grids as well as grids represented by both graded and non-graded quadtrees/octrees.
 588 The interpolations are based on Moving Least Squares approximations per-
 589 formed to compute the weights of the final finite difference stencil, and incor-
 590 porated in the linear system matrix. We performed several convergence tests
 591 for a simple Poisson equation in graded and non-graded grids, with 2nd order
 592 convergence for both the solution and its gradient. Comparisons with other
 593 already published methods provide evidence of the superiority and flexibility of
 594 our technique. We further extended this methodology to compute the solution of
 595 the incompressible Navier-Stokes equations. After testing the robustness of our
 596 methodology with several academic tests involving the Helmholtz-Hodge decom-
 597 position, we presented convergence tests for incompressible flows with manufac-

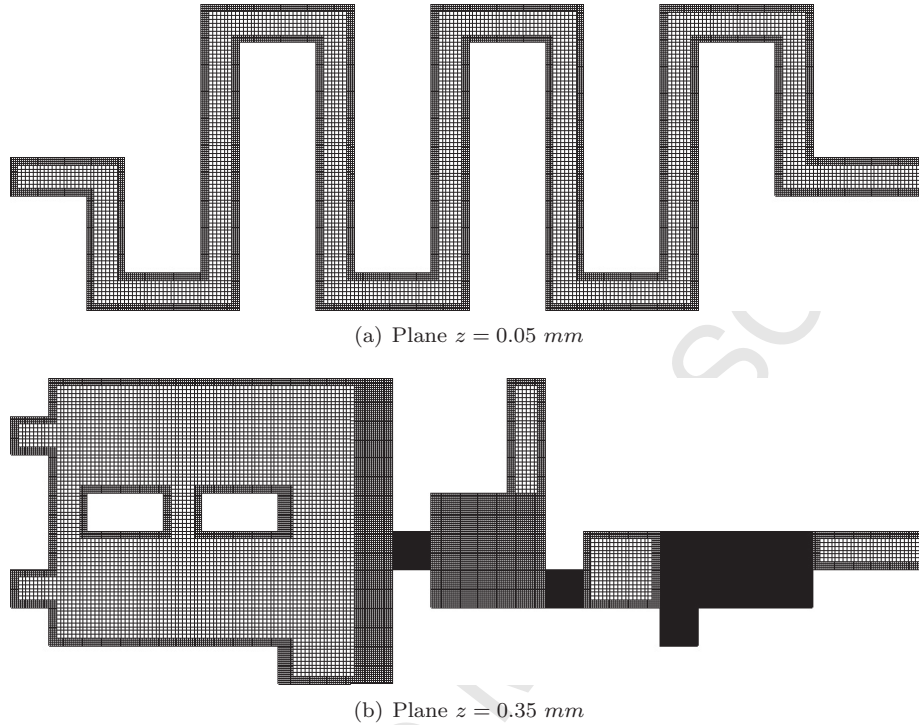


Figure 17: Slices showing details of the octree mesh used to discretize the 3D array of microchannels.

598 tured solutions in both 2D and 3D, computed in graded and non-graded grids.
 599 The results are consistent with previous tests, yielding 2nd order convergence
 600 for the primitive variables. Finally, the incompressible flow of a single fluid in
 601 a three-dimensional array of microchannels is simulated, introducing a level of
 602 complexity to the geometry of the domain, together with a locally-refined grid.
 603 The developed method handles this simulation seamlessly, yielding reasonable
 604 qualitative results. Future work will focus on the extension of this methodology
 605 for non-Newtonian fluid models, as well as multi-fluid flows.

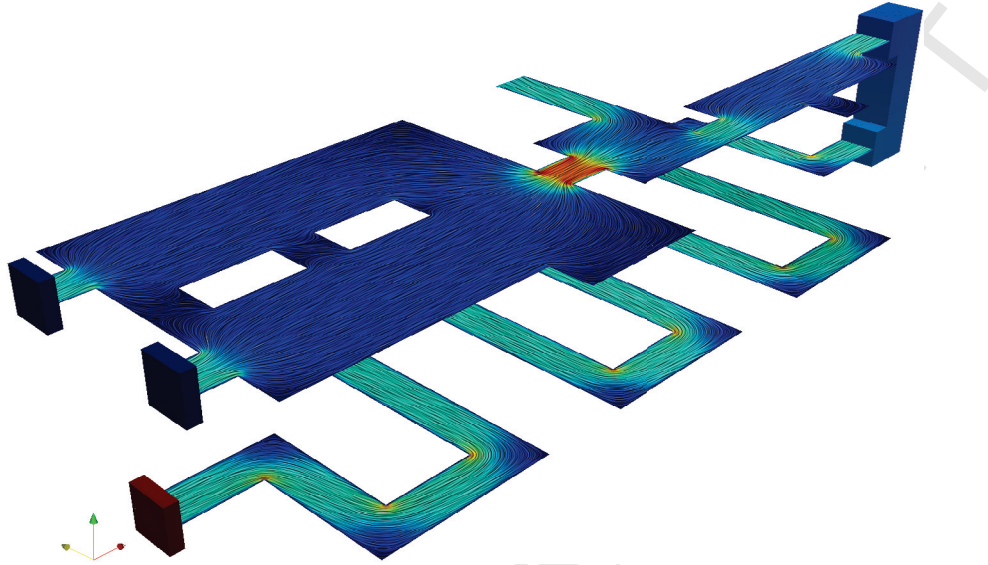


Figure 18: Streamlines for the complex 3D array of channels, taken from two slices, $z = 0.05 \text{ mm}$ and $z = 0.35 \text{ mm}$. The color scale varies from smallest (blue) to largest (red) velocity magnitude.

606 Acknowledgments

607 All authors thank the financial support from Brazilian Petroleum Agency
 608 (ANP)/Petrobras grant 0050.0075367.12.9, and from the São Paulo Research
 609 Foundation (FAPESP) grant 2013/07375-0. J.L. Ansoni and A. Castelo also
 610 thanks the financial support from the National Council for Scientific and Tech-
 611 nological Development (CNPq) grants 152397/2016-7 and 307483/2017-7. This
 612 study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal
 613 de Nível Superior - Brazil (CAPES) Finance Code 001.

614 References

- 615 [1] S. Popinet, “Gerris: a tree-based adaptive solver for the incompressible
 616 Euler equations in complex geometries,” *Journal of Computational Physics*,
 617 vol. 190, pp. 572–600, Sept. 2003.

- 618 [2] F. Losasso, F. Gibou, and R. Fedkiw, “Simulating water and smoke with
619 an octree data structure,” *ACM Trans. Graph.*, vol. 23, pp. 457–462, Aug.
620 2004.
- 621 [3] F. Losasso, R. Fedkiw, and S. Osher, “Spatially adaptive techniques for
622 level set methods and incompressible flow,” *Computers & Fluids*, vol. 35,
623 pp. 995–1010, dec 2006.
- 624 [4] C. Min and F. Gibou, “A second order accurate projection method for
625 the incompressible Navier-Stokes equations on non-graded adaptive grids,”
626 *Journal of Computational Physics*, vol. 219, pp. 912–929, 2006.
- 627 [5] A. Guittet, M. Theillard, and F. Gibou, “A stable projection method for the
628 incompressible Navier-Stokes equations on arbitrary geometries and adap-
629 tive quad/octrees,” *Journal of Computational Physics*, vol. 292, pp. 215–
630 238, July 2015.
- 631 [6] F. Gibou, R. Fedkiw, and S. Osher, “A review of level-set methods and some
632 recent applications,” *Journal of Computational Physics*, vol. 353, pp. 82–
633 109, jan 2018.
- 634 [7] P. Gómez, C. Zanzi, J. López, and J. Hernández, “Simulation of high den-
635 sity ratio interfacial flows on cell vertex/edge-based staggered octree grids
636 with second-order discretization at irregular nodes,” *Journal of Computa-
637 tional Physics*, vol. 376, pp. 478–507, jan 2019.
- 638 [8] M. J. Berger and J. Olinger, “Adaptive mesh refinement for hyperbolic
639 partial differential equations,” *Journal of Computational Physics*, vol. 53,
640 no. 3, pp. 484–512, 1984.
- 641 [9] L. H. Howell and J. B. Bell, “An adaptive-mesh projection method for

- 642 viscous incompressible flow,” *SIAM J. SCI. COMPUT.*, vol. 18, pp. 18–
643 996, 1996.
- 644 [10] M. R. Pivello, M. M. Villar, R. Serfaty, A. M. Roma, and A. Silveira-Neto,
645 “A fully adaptive front tracking method for the simulation of two phase
646 flows,” *International Journal of Multiphase Flows*, vol. 58, pp. 72–82, 2014.
- 647 [11] A. M. Khokhlov, “Fully threaded tree algorithms for adaptive refinement
648 fluid dynamics simulations,” *Journal of Computational Physics*, vol. 143,
649 no. 2, pp. 519–543, 1998.
- 650 [12] C. Batty, “A cell-centred finite volume method for the Poisson problem
651 on non-graded quadtrees with second order accurate gradients,” *Journal of*
652 *Computational Physics*, vol. 331, pp. 49–72, Feb. 2017.
- 653 [13] M. A. Olshanskii, K. M. Terekhov, and Y. V. Vassilevski, “An octree-
654 based solver for the incompressible Navier-Stokes equations with enhanced
655 stability and low dissipation,” *Computers & Fluids*, vol. 84, pp. 231 – 246,
656 2013.
- 657 [14] C. Min, F. Gibou, and H. D. Ceniceros, “A supra-convergent finite dif-
658 ference scheme for the variable coefficient Poisson equation on non-graded
659 grids,” *Journal of Computational Physics*, vol. 218, pp. 123–140, Oct. 2006.
- 660 [15] T. Belytschko, Y. Krongauz, D. Organ, M. Fleming, and P. Krysl, “Mesh-
661 less methods: An overview and recent developments,” *Computer Methods*
662 *in Applied Mechanics and Engineering*, vol. 139, no. 1, pp. 3–47, 1996.
- 663 [16] J. J. Benito, F. Ureña, and L. Gavete, “Influence of several factors in
664 the generalized finite difference method,” *Applied Mathematical Modelling*,
665 vol. 25, pp. 1039–1053, Dec. 2001.

- 666 [17] S. Li and W. K. Liu, “Meshfree and particle methods and their applica-
667 tions,” *Appl Mech Rev*, vol. 55, no. 1, pp. 1–34, 2002.
- 668 [18] X. K. Zhang, K.-C. Kwon, and S.-K. Youn, “The least-squares meshfree
669 method for the steady incompressible viscous flow,” *Journal of Computa-
670 tional Physics*, vol. 206, pp. 182–207, June 2005.
- 671 [19] V. P. Nguyen, T. Rabczuk, S. Bordas, and M. Duflot, “Meshless meth-
672 ods: A review and computer implementation aspects,” *Mathematics and
673 Computers in Simulation*, vol. 79, pp. 763–813, Dec. 2008.
- 674 [20] B. Seibold, “Minimal positive stencils in meshfree finite difference methods
675 for the Poisson equation,” *Computer Methods in Applied Mechanics and
676 Engineering*, vol. 198, pp. 592–601, Dec. 2008.
- 677 [21] X. Zheng, W.-y. Duan, and Q.-W. Ma, “Comparison of improved meshless
678 interpolation schemes for SPH method and accuracy analysis,” *Journal of
679 Marine Science and Application*, vol. 9, no. 3, pp. 223–230, 2010.
- 680 [22] H. Ding, C. Shu, K. S. Yeo, and D. Xu, “Simulation of incompressible
681 viscous flows past a circular cylinder by hybrid FD scheme and meshless
682 least square-based finite difference method,” *Computer Methods in Applied
683 Mechanics and Engineering*, vol. 193, pp. 727–744, Mar. 2004.
- 684 [23] H. Ding, C. Shu, and Q. D. Cai, “Applications of stencil-adaptive finite
685 difference method to incompressible viscous flows with curved boundary,”
686 *Computers & Fluids*, vol. 36, pp. 786–793, May 2007.
- 687 [24] C. S. Chew, K. S. Yeo, and C. Shu, “A generalized finite-difference (GFD)
688 ALE scheme for incompressible flows around moving solid bodies on hy-
689 brid meshfree-cartesian grids,” *Journal of Computational Physics*, vol. 218,
690 pp. 510–548, Nov. 2006.

- 691 [25] X. Y. Wang, K. S. Yeo, C. S. Chew, and B. C. Khoo, “A SVD-GFD scheme
692 for computing 3D incompressible viscous fluid flows,” *Computers & Fluids*,
693 vol. 37, pp. 733–746, July 2008.
- 694 [26] A. Quarteroni, R. Sacco, and F. Saleri, *Numerical Mathematics*. Springer,
695 2007.
- 696 [27] J. B. Perot, “An analysis of the fractional step method,” *Journal of Com-
697 putational Physics*, vol. 108, pp. 51–58, 1993.
- 698 [28] J. L. Guermond and L. Quartapelle, “On stability and convergence of pro-
699 jection methods based on pressure Poisson equation,” *International Journal
700 for Numerical Methods in Fluids*, 1998.
- 701 [29] J. L. Guermond, P. Mineev, and J. Shen, “An overview of projection meth-
702 ods for incompressible flows,” *Computer Methods in Applied Mechanics and
703 Engineering*, vol. 195, no. 44-47, pp. 6011–6045, 2006.
- 704 [30] P. Gervasio and F. Saleri, “Algebraic fractional-step schemes for time-
705 dependent incompressible Navier-Stokes equations,” *J. Sci. Comput.*,
706 vol. 27, pp. 257–269, 2006.
- 707 [31] F. S. Sousa, C. M. Oishi, and G. C. Buscaglia, “Spurious transients of pro-
708 jection methods in microflow simulations,” *Computer Methods in Applied
709 Mechanics and Engineering*, vol. 285, pp. 659–693, 2015.
- 710 [32] R. Codina, “Pressure stability in fractional step finite element methods for
711 incompressible flows,” *Journal of Computational Physics*, vol. 170, no. 1,
712 pp. 112–140, 2001.
- 713 [33] A. Quarteroni, F. Saleri, and A. Veneziani, “Factorization methods for the
714 numerical approximation of Navier-Stokes equations,” *Computer methods
715 in applied mechanics and engineering*, vol. 188, no. 1-3, pp. 505–526, 2000.

- 716 [34] A. J. Chorin, “Numerical solution of the Navier-Stokes equations,” *Math-*
717 *ematics of Computation*, vol. 22, pp. 745–762, 1968.
- 718 [35] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman,
719 L. Dalcin, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C.
720 McInnes, K. Rupp, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang,
721 “PETSc users manual,” Tech. Rep. ANL-95/11 - Revision 3.7, Argonne
722 National Laboratory, 2016.
- 723 [36] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman,
724 L. Dalcin, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C.
725 McInnes, K. Rupp, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang,
726 “PETSc Web page,” 2016.
- 727 [37] T. M. Shih, C. H. Tan, and B. C. Hwang, “Effects of grid staggering on nu-
728 merical schemes,” *International Journal for Numerical Methods in Fluids*,
729 vol. 9, no. 2, pp. 193–212, 1989.