An energy-preserving unconditionally stable fractional step method on collocated grids

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05-09 June 2022, ECCOMAS 2022, Oslo, Norway

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1. Motivation of this work

Motivation: Is it possible to find an energy-preserving unconditionally stable fractional step method on collocated grids for any mesh?

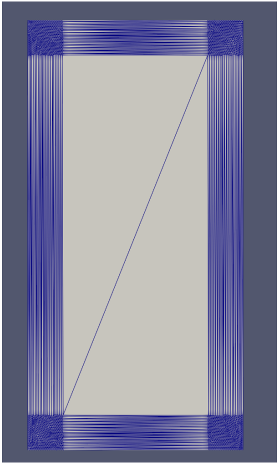

Figure 1: Example of a highly distorted mesh.

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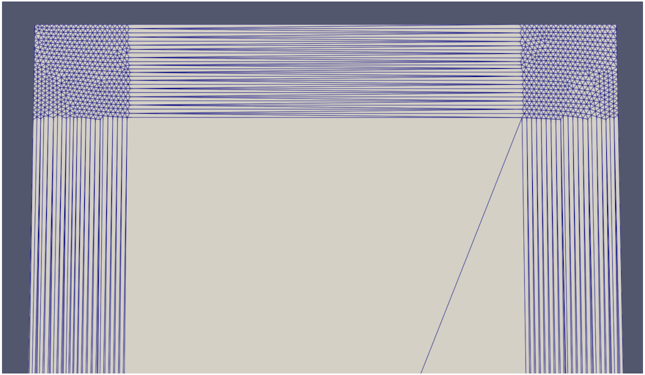

Figure 2: Zoom of the top part of the previous mesh.

2. Definition of basic collocated operators

Incompressible NS equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \frac{1}{Re}\Delta \mathbf{u} - \nabla p, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (2)$$

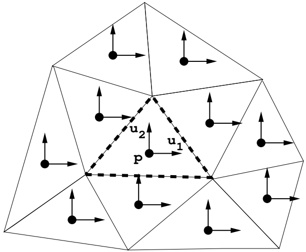

Figure 3: General unstrucured mesh.

Definition of basic collocated operators

Let us suppose we have n control volumes and m faces.

Finite volume discretization of incompressible NS equations on an arbitrary collocated mesh

$$\Omega \frac{d\mathbf{u}_c}{dt} + C(\mathbf{u}_s)\mathbf{u}_c = -D\mathbf{u}_c - \Omega G_c \mathbf{p}_c, \quad (3)$$

$$M\mathbf{u}_s = \mathbf{0}_c. \quad (4)$$

- $\mathbf{p}_c = (p_1, ..., p_n)^T \in \mathbb{R}^n$ is the cell-centered pressure.
- $\mathbf{u}_c = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)^T \in \mathbb{R}^{3n}$, where $\mathbf{u}_i = ((u_i)_1, ..., (u_i)_n)^T$ are the vectors containing the velocity components corresponding to the x_i-spatial direction.
- $\mathbf{u}_s = ((u_s)_1, ..., (u_s)_m)^T \in \mathbb{R}^m$ is the staggered velocity.
- The velocities are related via the interpolator from cells to faces $\Gamma_{c\to s} \in \mathbb{R}^{m\times 3n} \implies \mathbf{u}_s = \Gamma_{c\to s}\mathbf{u}_c$.

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The (volumetric) interpolator from cells to faces can be constructed as follows:

$$\Gamma_{c \rightarrow s} = N\Pi, \tag{5}$$

where

- $N = (N_{s,x} N_{s,y} N_{s,z}) \in \mathbb{R}^{m \times 3m}$ where $N_{s,x}, N_{s,y}, N_{s,z} \in \mathbb{R}^{m \times m}$ are diagonal matrices containing the x_i spatial component of the face normal vectors.
- $\Pi = I_3 \otimes \Pi_{c \rightarrow s} \in \mathbb{R}^{3m \times 3n}$.
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Definition of basic collocated operators

- $\Omega_c \in \mathbb{R}^{n\times n}$ is a diagonal matrix with the cell-centered volumes $\implies \quad \Omega = I_3 \otimes \Omega_c$.
- $C_c(\mathbf{u}_s) \in \mathbb{R}^{n\times n}$ is the cell-centered convective operator for a discrete scalar field $\implies \quad C(\mathbf{u}_s) = I_3 \otimes C_c(\mathbf{u}_s)$.
- $D_c \in \mathbb{R}^{n\times n}$ is the cell-centered diffusive operator for a discrete scalar field $\implies \quad D = I_3 \otimes D_c$.

Finally,

- $G_c \in \mathbb{R}^{3n\times n}$ represents the discrete collocated gradient.
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Other useful operators

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\begin{aligned}
\boxed{G = -\Omega_s^{-1} M^T,} \\
L = MG = -M\Omega_s^{-1} M^T, \\
L_c = M_c G_c = -M\Gamma_{c\to s}\Omega^{-1}\Gamma_{c\to s}^T M^T, \\
\Gamma_{s\to c} = \Omega^{-1}\Gamma_{c\to s}^T \Omega_s.
\end{aligned}
\qquad (6)
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where G is the center-to-face staggered gradient, L is the Laplacian operator, L_c is the collocated-Laplacian operator and $\Gamma_{s\to c}$ is the face-to-cell interpolator.

For more information about Symmetry-Preserving discretization consult: *F.X. Trias, O. Lehmkuhl, A. Oliva, C.D. Perez-Segarra, and R.W.C.P. Verstappen. Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured meshes. Journal of Computational Physics, 258:246–267, 2014.*

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3. Conservation of global kinetic energy

Global kinetic energy equation

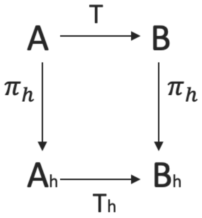
$$\frac{d||\mathbf{u}_c||^2}{dt} = -\mathbf{u}_c^T(C(\mathbf{u}_s) + C^T(\mathbf{u}_s))\mathbf{u}_c - \mathbf{u}_c^T(D + D^T)\mathbf{u}_c - \mathbf{u}_c^T \Omega G_c \mathbf{p}_c - \mathbf{p}_c^T G_c^T \Omega^T \mathbf{u}_c. \quad (7)$$

In absence of diffusion, that is $D = 0$, the global kinetic energy is conserved if:

- $C(\mathbf{u}_s) = -C^T(\mathbf{u}_s)$, i.e, the convective operator should be skew-symmetric.
- $(-\Omega G_c)^T = M\Gamma_{c\to s}$, because $M\mathbf{u}_s = \mathbf{0}_c$.

Question: Can we find a mathematical reason to justify these relations, instead of a physical one?

Mimicking continuos properties



- A and B are two vectorial spaces.
- π_h is a discretization operator.
- T is a continuous operator.
- A_h, B_h and T_h are the discrete counterparts of A, B and T, respectively.

We will require this diagram to be commutative.

Mimicking continuos properties: relation between gradient and divergence operators

- From a continuos level, the adjoint operator of the divergence is the gradient:

$$< \nabla \cdot a | b > = - < a | \nabla b >, \tag{8}$$

where $< a|b > = \int_\Omega abdV$ represents the inner product of functions. The discrete counterpart of the inner product is $< a_h | b_h >_\Omega = a_h^T \Omega b_h$.

- Applying π_h to (8) we obtain:

$$< \Omega_1^{-1} M a_h | b_h >_{\Omega_1} = - < a_h | G b_h >_{\Omega_2} . \tag{9}$$

If $\Omega_1 = \Omega$ and $\Omega_2 = \Omega_s$, then:

$$G = -\Omega_s^{-1} M^T. \tag{10}$$

- Finally, from the skew-symmetry of the continuos convective operator follows that $C(u_s)$ should be skew-symmetric.

4. A stable pressure gradient interpolation

Solving 1D NS equations with a fractional step method interpolating the pressure gradient with a mid-point scheme (checkerboard is not corrected):

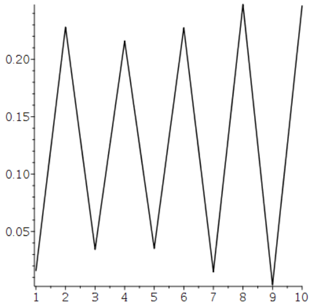


Figure 4: Vel. for max. aspect ratio 1 (mid-point scheme)

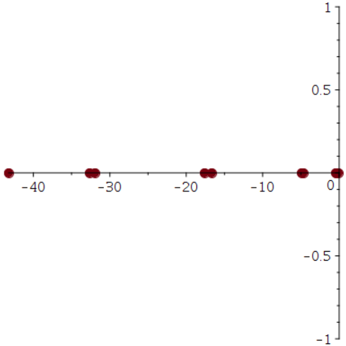


Figure 5: Eigenvalues of $L - L_c$

A stable pressure gradient interpolation

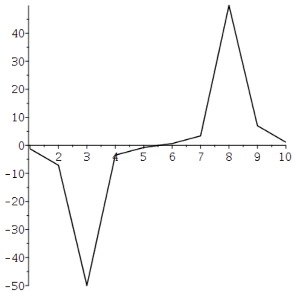


Figure 6: Vel. for max. aspect ratio 20 (mid-point scheme)

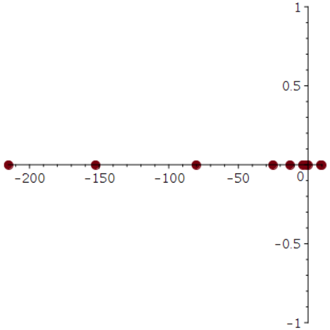


Figure 7: Eigenvalues of $L - L_c$

A stable pressure gradient interpolation

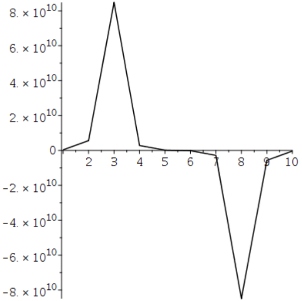


Figure 8: Vel. for max. aspect ratio 40 (mid-point scheme)

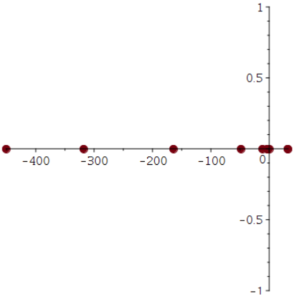


Figure 9: Eigenvalues of $L - L_c$

A stable pressure gradient interpolation

- **Mid-point scheme:** $\phi_f = \frac{1}{2}(\phi_{c1} + \phi_{c2})$.
- **Volume weighted scheme:** $\phi_f = \frac{V_{s1}}{V_{s1}+V_{s2}}\phi_{c1} + \frac{V_{s2}}{V_{s1}+V_{s2}}\phi_{c2}$.

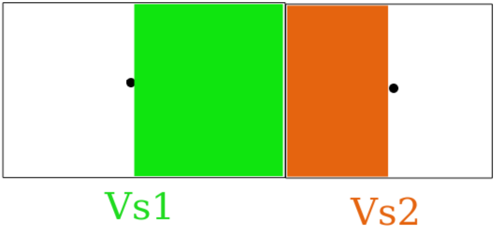


Figure 10: Volume weighted volumes

A stable pressure gradient interpolation

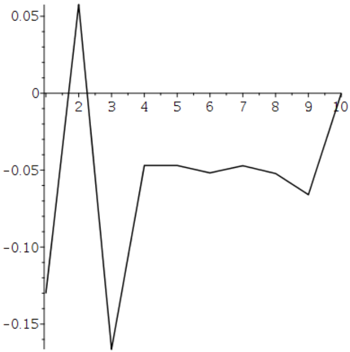


Figure 11: Vel. for max. aspect ratio 40 (volume weighted scheme)

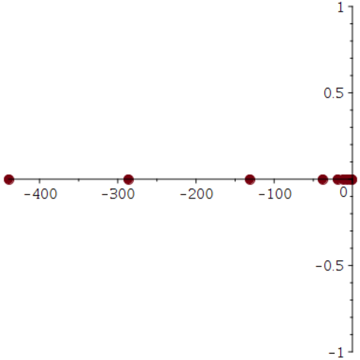


Figure 12: Eigenvalues of $L - L_c$

FSM iterative Poisson equation in collocated meshes

$$L\tilde{p}_c^{n+1} = M_c u_c^n \quad \longrightarrow \quad u_c^{n+1} = u_c^n - G_c \tilde{p}_c^{n+1}, \tag{11}$$

where $M_c = M\Gamma_{c\rightarrow s}$and $G_c = \Gamma_{s\rightarrow c} G = -\Omega_c^{-1}\Gamma_{c\rightarrow s}^T M^T$ are the collocated divergence and the collocated gradient. Developing the correction in u_c^n:

$$u_c^n = u_c^{n-1} - G_c\tilde{p}_c^n = u_c^{n-2} - G_c\tilde{p}_c^n - G_c\tilde{p}_c^{n-1} = \cdots = u_c^p - G_c \sum_{i=1}^{n} \tilde{p}_c^i \tag{12}$$

So, the acumulated pressure at n iteration is:

$$p_c^n = \sum_{i=1}^{n} \tilde{p}_c^i \tag{13}$$

Introducing all this in (7) we obtain:

$$Lp_c^{n+1} = M\Gamma_{c\rightarrow s} u_c^p + (L - L_c)p_c^n. \tag{14}$$

A stable pressure gradient interpolation

- In order to obtain stable solutions, we require the eigenvalues of $L - L_c$ to be negative.
- This can be achieved by using the volume weighted scheme:

$$\Pi_{c \rightarrow s} = \Delta_s^{-1} \Delta_{sc}^T, \tag{15}$$

  where $\Delta_s \in \mathbb{R}^{m \times m}$ is a diagonal matrix containing the projected distances between two adjacent control volumes, and $\Delta_{sc} \in \mathbb{R}^{m \times n}$ is a matrix containing the projected distances between an adjacent cell node and its corresponding face.
- It is relatively easy to prove it for cartesian meshes and their stretchings, but it is not easy to prove for a general triangular mesh.

This problem was widely adressed in: *D. Santos, J. Muela, N. Valle, F.X. Trias, On the Interpolation Problem for the Poisson Equation on Collocated Meshes. 14th WCCM-ECCOMAS Congress 2020, DOI: 10.23967/wccm-eccomas.2020.257.*

Invariance of definiteness

Motivation: It is easy to prove that a Cartesian mesh meet the previous criteria, but it is not easy to prove it for rotated Cartesian meshes.

Result 4

The definiteness of $L - L_c$ is invariant under rotations of the mesh.

- The face-normal vectors are contained in the matrix N.
- A generalized rotation matrix R can be constructed in order to change properly the matrix N.
- As N is inside $\Gamma_{c \rightarrow s}$ (which is inside L_c), changing the basis will lead us to a new volumetric interpolator $\Gamma_{c \rightarrow s}^{new}$.

5. Air-filled differentially heated cavity for extremely distorted unstructured meshes

In order to check the stability of the method, some tests have been carried out with very coarse and very bad quality meshes. Here, a differentially heated cavity test is presented:

- Air-filled (Pr $= 0.71$).
- Aspect ratio 2.
- Rayleigh number (based on the cavity height) of 10^6.

The symmetries of the operators have been respected and a volume weighted interpolator was used to interpolate the pressure gradient.

Remark: Using a mid point scheme will blow up the simulation at the beginning.

Air-filled differentially heated cavity for extremely distorted unstructured meshes

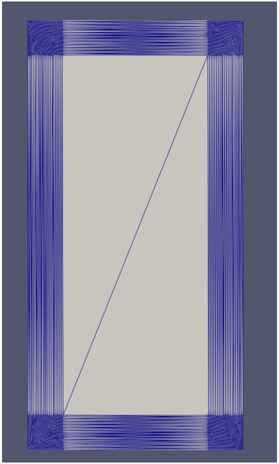


Figure 13: Mesh used to run the case.

Air-filled differentially heated cavity for extremely distorted unstructured meshes.

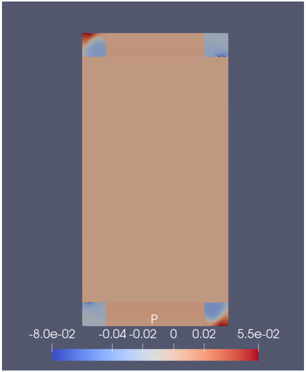


Figure 14: Pressure distribution.

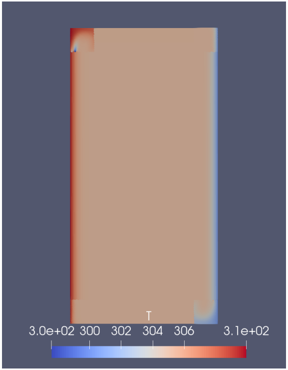


Figure 15: Temperature distribution.

Air-filled differentially heated cavity for extremely distorted unstructured meshes.

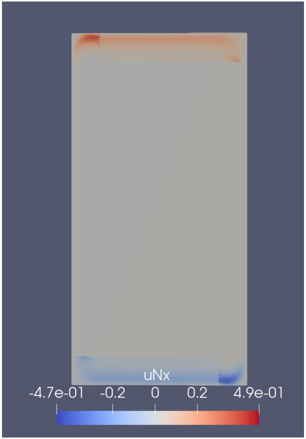


Figure 16: Velocity distribution in x-direction.

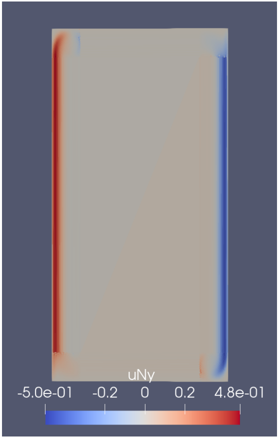


Figure 17: Velocity distribution in y-direction.

6. Conclusions

- An energy-preserving unconditionally stable fractional step method on collocated grids has been presented.
- There are mathematical reasons beyond physical ones in order to preserve the underlying symmetries of the differential operators.
- The appearance of unphysical velocities is a common problem found in highly distorted meshes, and it commes from the interpolation of the pressure gradient in the velocity correction.
- The volume weighted scheme solves this problem for Cartesian meshes.
- For unstructured triangular meshes, it seems that it can be also stable. At least, it is much more stable than a mid-point interpolation.