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Numerical Analysis

A fractional step method based on a pressure Poisson equation for incompressible flows with variable density

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Abstract

A new fractional time technique for solving incompressible flows with variable density is proposed. The main feature of the method is that, as opposed to other known algorithms, the pressure is computed by solving a Poisson equation, which greatly reduces the computational cost. The method is proved to be stable and is numerically illustrated. ***To cite this article: J.-L. Guermond, A. Salgado, C. R. Acad. Sci. Paris, Ser. I 346 (2008).***

Résumé

Une technique de pas fractionnaire basée sur une équation de Poisson pour les fluides incompressibles à densité variable. Nous proposons une famille d'algorithmes à pas fractionnaire basés sur une équation de Poisson pour l'approximation des fluides incompressibles à densité variable. On démontre que la méthode est stable. ***Pour citer cet article : J.-L. Guermond, A. Salgado, C. R. Acad. Sci. Paris, Ser. I 346 (2008).***

Version française abrégée

L'objectif de cette Note est d'introduire une famille d'algorithmes à pas fractionnaires pour l'approximation des équations de Navier–Stokes incompressible à densité variable (1), (2).

Les méthodes de pas fractionnaires consitent à remplacer à chaque pas de temps la résolution d'un problème de Stokes généralisé par deux sous-problèmes où la vitesse et la pression sont découplés. Les méthodes de pas fractionnaires usuelles sont toutes basées sur une étape de projection conduisant à résoudre un problème du second ordre à coefficients variables du type (3), voir e.g. [1,2,7,9]. Le problème (3) est elliptique et ne présente pas vraiment de difficulté théorique ; toutefois, il doit être assemblé et preconditionné à chaque pas de temps, ce qui peut être coûteux. Nous proposons dans cette Note une famille d'algorithmes à pas fractionnaires où (3) est remplacé par un problème de Poisson, rendant ainsi la méthode de résolution très rapide car l'assemblage et le préconditionnement ne sont faits qu'une seule fois.

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Le point de départ de l'argument est la version incrémentale de l'algorithme de correction de pression pour les fluides incompressibles à densité constante, voir e.g. [6,10]. (C'est une version plus précise de l'algorithme non incrémental de Chorin–Temam [3,11].) Comme remarqué dans [4,6], la vitesse solénoidale (i.e., la vitesse projetée) peut être complètement éliminée de l'algorithme. Après élimination, l'algorithme résultant correspond à l'approximation de (4) où le pas de temps est remplacé par ϵ. Formellement (4) est une perturbation d'ordre $\mathcal{O}(\epsilon^2)$ de (1), et c'est pour cette raison que la version incrémentale de l'algorithme de correction de pression est formellement précis à l'ordre deux lorsque la densité est constante.

L'idée sur laquelle repose le nouvel algorithme présenté dans cette Note est d'utiliser la perturbation (4) aussi pour les fluides à densité variable.

Soit Δt le pas de temps et posons $t^n := n\Delta t$, $n = \overline{0, N-1}$, $T := N\Delta t$. On choisit maintenant un réel positif χ dans l'intervalle $(0, \rho_{\min}]$, i.e., $\chi \in (0, \rho_{\min}]$, et on définit $\epsilon := \Delta t/\chi$. Dans les applications numériques rapportées à la fin de la Note nous avons pris $\chi = \rho_{\min} := \min_{\mathbf{x}\in\Omega} \rho_0(x) > 0$. En approchant la dérivée temporelle de la vitesse dans (4) par un quotient différentiel d'orde un, on obbtient l'algorithme (5)–(6)–(7)–(8). La pricipale caractéristique de cet algorithme est que (7) est un problème de Poisson, qui peut-être résolu rapidement contrairement à (3). Nous ne détaillons pas comment réaliser (5), mais il suffit en général d'utiliser un algorithme monotone. Le principal résultat de cette Note est le Théorème 3.1. C'est à notre connaissance le premier résultat de stabilité connu pour un algorithme à pas fractionnaire basé sur un problème de Poisson pour des fluides incompressibles à densité variable. On peut démontrer le même type de résultat (Corollaire 4.1) pour l'algorithme totalement discrétisé (10)–(13), pourvu que les espaces discrets soient conformes et que la condition LBB soit satisfaite.

Une version formellement d'ordre deux de la méthode est obtenue en approchant la dérivée temporelle de la vitesse dans (4) par le schéma d'orde deux à trois pas, BDF2 : (14)–(17). La correction de pression (17) correspond à la version rotationnelle de (4) pour laquelle $\epsilon p_t = \phi - \mu\nabla\cdot\mathbf{u}$. C'est pour cette version de la correction de pression que les meilleurs résultats de convergence connus actuellement on été prouvés lorsque la densité est constante, [8]. Bien que les tests numériques montrent que (14)–(17) est stable et convergent, nous n'avons pas encore pu établir ce résultat. Les illustrations numériques de la section 6 ont été obtenus avec (14)–(17).

1. Introduction

This Note deals with the numerical approximation of incompressible viscous flows with variable density:

$$\begin{cases} \rho_t + \nabla\cdot(\rho\mathbf{u}) = 0, \\ \rho(\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u}) + \nabla p - \mu\Delta\mathbf{u} = \mathbf{f}, \\ \nabla\cdot\mathbf{u} = 0, \end{cases} \tag{1}$$

where the dependent variables are the density $\rho > 0$, the velocity field $\mathbf{u}$, and the pressure p. The constant μ is the dynamic viscosity coefficient and $\mathbf{f}$ is a driving external force. The fluid occupies a bounded domain Ω in $\mathbb{R}^d$ (with $d = 2$ or 3) and a solution to the above problem is sought over a time interval $[0, T]$. The system is supplemented by the following initial and boundary conditions for $\mathbf{u}$ and ρ:

$$\rho(x, 0) = \rho_0(x), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, t)|_\Gamma = \mathbf{b}(\mathbf{x}, t), \tag{2}$$

where $\Gamma = \partial\Omega$. Throughout this Note we assume that the boundary Γ is impermeable, i.e., $\mathbf{u}\cdot\mathbf{n} = 0$ everywhere on Γ. We henceforth assume that $\rho_{\min} := \min_{\mathbf{x}\in\Omega} \rho_0(x) > 0$, i.e., there is no vacuum.

Approximating the coupled system (1), (2) is computer intensive due to the elliptic character induced by incompressibility. Once time is discretized and the velocity/pressure coupling is retained, (1) reduces to solving a generalized Stokes problem at each time step. Alternative strategies for solving (1) consists of un-coupling the velocity and the pressure by using fractional time-stepping algorithms, see for example [1,2,7,9]. The goal of the present Note is to introduce and analyze one of these methods.

The common feature of all the current fractional time-stepping methods is that at each time step, say t^{n+1}, the pressure or some related scalar quantity, say Φ, must be evaluated by solving an equation of the following form:

$$-\nabla\cdot\left((\rho^{n+1})^{-1}\nabla\Phi\right) = \Psi, \qquad \partial_n\Phi|_\Gamma = 0, \tag{3}$$

where ρ^{n+1} is an approximation of the density at time t^{n+1} and ψ is some right-hand side that varies at each time step. Solving (3) can be time consuming since it requires assembling and pre-conditioning a variable coefficient stiffness matrix at each time step.

The objective of the present Note is to introduce a fractional time-stepping methods for solving variable density flows that involve solving only one Poisson problem per time step instead of problems like (3). The proposed algorithm is proved to be stable and illustrated numerically.

2. The heuristics

The starting point is the incremental pressure-correction algorithm for constant density flow, see e.g. [6,10]. (This algorithm is a more accurate version of the so-called Chorin–Temam method [3,11].) The method consists of computing two sequences of approximate velocities $(\tilde{\mathbf{u}}^{n+1})_{n>0}$, $(\mathbf{u}^{n+1})_{n>0}$, and one sequence of approximate pressure $(p^{n+1})_{n\geqslant 0}$. Each time step is decomposed into three sub-steps: The velocity $\tilde{\mathbf{u}}^{n+1}$ is computed at the first sub-step by making the pressure explicit; $\tilde{\mathbf{u}}^{n+1}$ is then projected onto the solenoidal vector fields with zero normal trace, the result being $\mathbf{u}^{n+1}$; the pressure is corrected at the last sub-step.

As emphasized in [4,6], the so-called projected velocity $\mathbf{u}^{n+1}$ can be algebraically eliminated from the algorithm and once this is done and difference quotients are replaced by time derivatives and the remaining Δt is replaced by ϵ, the above algorithm reduces to the following perturbation of the Navier–Stokes equations:

$$\begin{cases} \rho(\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u}) + \nabla p - \mu\Delta\mathbf{u} = \mathbf{f}, & \mathbf{u}|_\Gamma = 0, \quad \mathbf{u}|_{t=0} = \mathbf{u}_0, \\ \nabla\cdot\mathbf{u} - \frac{\epsilon}{\rho}\Delta\phi = 0, & \partial_n\phi|_\Gamma = 0, \\ \epsilon p_t = \phi. \end{cases} \tag{4}$$

Formally (4) is a $\mathcal{O}(\epsilon^2)$ perturbation of the constant density incompressible Navier–Stokes equations. We are now going to use (4) as the starting point for a new algorithm for variable density flows.

3. A new algorithm

Let Δt be a time step and set $t^n := n\Delta t$, $n = \overline{0, N-1}$, $T := N\Delta t$. Choose $\chi \in \mathbb{R}^+$ in the interval $(0, \rho_{\min}]$, i.e., $\chi \in (0, \rho_{\min}]$, and set $\epsilon := \Delta t/\chi$. In the computations reported at the end of the Note we take $\chi = \rho_{\min}$.

The new algorithm consists of discretizing (4) and proceeds as follows: Set $\rho^0 = \rho_0$, $\mathbf{u}^0 = \mathbf{u}_0$, and $\phi^0 = 0$. Let p_0 be the pressure at $t = 0$ and set $p^0 = p_0$. This quantity can be deduced from ρ^0 and $\mathbf{u}_0$. For instance if the flow is at rest at $t = 0$, then $p_0 = 0$. Then, given $(\rho^n, \mathbf{u}^n, p^n, \phi^n)$, $n = \overline{0, N-1}$, the density is updated as follows:

$$\text{Compute } \rho^{n+1} \text{ so that } \begin{cases} \{\rho^n\}_{n=\overline{0,N}} \text{ is uniformly bounded in } L^\infty(\Omega) \\ \forall n = \overline{0, N}, \quad \chi \leqslant \rho^n(x), \text{ a.e. in } \Omega. \end{cases} \tag{5}$$

Setting $\mathbf{w}^\star := \rho^{n+1}\mathbf{u}^n$ and $p^\star := p^n + \phi^n$, the velocity is updated using

$$\frac{1}{\Delta t}\left[\frac{1}{2}(\rho^{n+1} + \rho^n)\mathbf{u}^{n+1} - \rho^n\mathbf{u}^n\right] + \mathbf{w}^\star\cdot\nabla\mathbf{u}^{n+1} + \frac{1}{2}\nabla\cdot(\mathbf{w}^\star)\mathbf{u}^{n+1} - \mu\Delta\mathbf{u}^{n+1} + \nabla p^\star = \mathbf{f}^{n+1}. \tag{6}$$

The pressure correction is updated using

$$\Delta\phi^{n+1} = \frac{\chi}{\Delta t}\nabla\cdot\mathbf{u}^{n+1}. \tag{7}$$

Finally, the pressure is updated by

$$p^{n+1} = p^n + \phi^{n+1}. \tag{8}$$

Remark 1. The hypotheses in (5) are rarely explicitly mentioned in numerical papers based on algorithms using (3), see e.g. [1,2,7,9], but it is required to guarantee well-posedness. It seems that these conditions are often overlooked. They can be achieved by using so-called monotone schemes. The numerical examples presented at the end of this paper have been computed using a shock-capturing technique for which we observed that the hypotheses in (5) are satisfied. The details of this shock-capturing technique will be reported elsewhere.

Remark 2. The pressure term in the momentum equation (6) is a second-order extrapolation of the pressure at time t^{n+1}, since, using (8) at time step n, we have $p^n + \phi^n = 2p^n - p^{n-1}$. The term $\frac{1}{\Delta t}[\frac{1}{2}(\rho^{n+1} + \rho^n)\mathbf{u}^{n+1} - \rho^n\mathbf{u}^n] + \frac{1}{2}\nabla\cdot(\rho^{n+1}\mathbf{u}^n)\mathbf{u}^{n+1}$ is asymptotically consistent with the equation. The purpose of this particular way of discretizing the quantity $\rho(\partial_t\mathbf{u})$ is to decouple the mass conservation and the momentum conservation equations.

The main result of this Note is the following:

Theorem 3.1. *Assume that the hypotheses in* (5) *hold. Then, setting* $\sigma^n = \sqrt{\rho^n}$, *for any* $\Delta t > 0$ *the solution to* (6)–(7)–(8) *satisfies*

$$\|\sigma^N \mathbf{u}^N\|^2 + 2\mu\Delta t \sum_{k=1}^{N} \|\nabla \mathbf{u}^k\|^2 + \frac{(\Delta t)^2}{\chi}\|\nabla p^N\|^2 + \frac{(\Delta t)^2}{\chi}\sum_{k=1}^{N-1}\left\|\nabla(p^k - p^{k-1})\right\|^2 \leqslant \|\sigma_0 \mathbf{u}_0\|^2 + \frac{(\Delta t)^2}{\chi}\|\nabla p_0\|^2.$$

To the best of our knowledge, Theorem 3.1 is the first known stability result for a fractional step technique based on a Poisson problem for variable density flows.

Remark 3. By analogy with projection methods for constant density flows [12,8], we can write a rotational version of the above algorithm by replacing the pressure update (8) by

$$p^{n+1} = p^n + \phi^{n+1} - \mu\nabla\cdot\tilde{\mathbf{u}}^{n+1}. \tag{9}$$

Although numerical tests (see below) reveal that the rotational version of algorithm (6)–(7)–(9) is stable and convergent, we have not yet been able to prove stability.

4. Space discretization

We now describe a conforming space discretization for the above algorithm. We assume that we have at hand families of finite-dimensional vectors spaces to approximate the velocity, the pressure, and the density fields, respectively. Say $\mathbf{X}_h \subset \mathbf{H}_0^1(\Omega)$, $M_h \subset H^1_{\int=0}(\Omega)$, $W_h \subset H^1(\Omega)$. The velocity space $\mathbf{X}_h$ and pressure space M_h are assumed to satisfy the so-called LBB condition.

We set $\rho_h^0 = \rho_{0h}$, $\mathbf{u}_h^0 = \mathbf{u}_{0h}$, $p_h^0 = p_{0h}$ and $\phi_h^0 = 0$ where $\rho_{0h} \in W_h$, $\mathbf{u}_{0h} \in \mathbf{X}_h$ and $p_{0h} \in M_h$ are suitable approximations of $\rho_0, \mathbf{u}_0$ and p_0, respectively. Then, the fully discretized algorithm proceeds as follows: Given $(\rho_h^n, \mathbf{u}_h^n, p_h^n, \phi_h^n) \in W_h \times \mathbf{X}_h \times M_h \times M_h$

$$\text{compute } \rho_h^{n+1} \text{ so that } \begin{cases} \{\rho_h^n\}_{n=\overline{0,N}} \text{ is uniformly bounded in } L^\infty(\Omega) \\ \forall n = \overline{0,N}, \quad \chi \leqslant \rho_h^n(x), \text{ a.e. in } \Omega. \end{cases} \tag{10}$$

Setting $\mathbf{w}_h^\star := \rho_h^{n+1}\mathbf{u}_h^n$ and $p_h^\star := p_h^n + \phi_h^n$, solve for $\mathbf{u}_h^{n+1} \in \mathbf{X}_h$ so that for all $\mathbf{v}_h \in \mathbf{X}_h$

$$\left\langle \frac{1}{2\Delta t}(\rho^{n+1} + \rho^n)\mathbf{u}_h^{n+1}, \mathbf{v}_h \right\rangle + \mu\langle\nabla\mathbf{u}_h^{n+1}, \nabla\mathbf{v}_h\rangle + d(\mathbf{w}_h^\star, \mathbf{u}_h^{n+1}, \mathbf{v}_h) = \left\langle \mathbf{f}^{n+1} - \nabla p_h^\star + \frac{1}{\Delta t}\rho_h^n\mathbf{u}_h^n, \mathbf{v}_h \right\rangle, \tag{11}$$

where $d(\mathbf{w}_h^\star, \mathbf{u}_h^{n+1}, \mathbf{v}_h) := \langle \mathbf{w}_h^\star\cdot\nabla\mathbf{u}_h^{n+1}, \mathbf{v}_h\rangle + \frac{1}{2}\langle\nabla\cdot(\mathbf{w}_h^\star)\mathbf{u}_h^{n+1}, \mathbf{v}_h\rangle$. Then solve for $\phi_n^{n+1} \in M_h$, so that

$$\langle\nabla\phi_h^{n+1}, \nabla q_h\rangle = \frac{\chi}{\Delta t}\langle\mathbf{u}_h^{n+1}, \nabla q_h\rangle, \quad \forall q_h \in M_h. \tag{12}$$

Finally, update the pressure $p_h^{n+1} \in M_h$ by solving

$$\langle p_h^{n+1}, q_h\rangle = \langle p_h^n + \phi_h^{n+1}, q_h\rangle, \quad \forall q_h \in M_h. \tag{13}$$

The stability hypotheses in (10) can be made to hold by using any suitably stabilized method: Galerkin-Least-Squares, Discontinuous-Galerkin, subgrid viscosity, method of characteristics and many others. The above algorithm is stable in the following sense:

Corollary 4.1. *Assume that* (10) *holds. Then, for any* $\Delta t > 0$ *the solution to* (11)–(12)–(13) *satisfies*

$$\|\sigma_h^N \mathbf{u}_h^N\|^2 + 2\mu\Delta t \sum_{k=1}^{N} \|\nabla \mathbf{u}_h^k\|^2 + \frac{(\Delta t)^2}{\chi}\|\nabla p_h^N\|^2 + \frac{(\Delta t)^2}{\chi}\sum_{k=1}^{N-1}\left\|\nabla(p_h^k - p_h^{k-1})\right\|^2$$
$$\leqslant \|\sigma_{0h}\mathbf{u}_{0h}\|^2 + \frac{(\Delta t)^2}{\chi}\|\nabla p_{0h}\|^2.$$

The proof of Corollary 4.1 is essentially the same as that of Theorem 3.1, since all the required test functions are admissible in the corresponding discrete spaces.

Remark 4. The above algorithm is an improvement over the second-order algorithm described in [9, Algorithm 2], which requires a strong (somewhat unrealistic) compatibility condition between the density and velocity spaces.

5. Second-order algorithm

We now propose a second-order rotational version of the above algorithm. The starting point is the BDF2 version of the rotational pressure-correction algorithm for constant density flows. The main idea consists of eliminating the so-called projected velocity and rewriting the projection step in the form of a Poisson equation where the constant density is replaced by χ. This program is realized as follows: first initialize $(\rho^0, \mathbf{u}^0, p^0, \phi^0)$ and $(\rho^1, \mathbf{u}^1, p^1, \phi^1)$. For instance $(\rho^1, \mathbf{u}^1, p^1, \phi^1)$ can be computed by using one step of the first-oder algorithm described above. Then for $n \geqslant 1$, introduce the linearly extrapolated velocity field at the new time level $n+1$ by defining $\mathbf{u}^\star = 2\mathbf{u}^n - \mathbf{u}^{n-1}$. The new density ρ^{n+1} is evaluated by solving the following discretized version of the mass conservation equation:

$$\frac{1}{2\Delta t}(3\rho^{n+1} - 4\rho^n + \rho^{n-1}) + \mathbf{u}^\star \cdot \nabla \rho^{n+1} = 0. \tag{14}$$

Similarly, the momentum equation is discretized in time as follows:

$$\frac{\rho^{n+1}}{2\Delta t}(3\mathbf{u}^{n+1} - 4\mathbf{u}^n + \mathbf{u}^{n-1}) + \rho^{n+1}(\mathbf{u}^\star \cdot \nabla)\mathbf{u}^{n+1} - \mu\Delta\mathbf{u}^{n+1} + \nabla\left(p^n + 2\phi^n - \frac{1}{2}\phi^{n-1}\right) = \mathbf{f}^{n+1}. \tag{15}$$

A pressure correction is evaluated by solving

$$\Delta\phi^{n+1} = \frac{3\chi}{2\Delta t}\nabla \cdot \mathbf{u}^{n+1}. \tag{16}$$

Finally, the pressure is updated by means of

$$p^{n+1} = p^n + \frac{3}{2}\phi^{n+1} - \mu\nabla \cdot \mathbf{u}^{n+1}. \tag{17}$$

Note that we did not add any particular extra stabilization terms in (14) and (15), the main reason being that the stability analysis of the method still eludes us at the moment; nevertheless, numerical experiments (see Section 6) show that this method is indeed stable and accurate.

6. Numerical illustrations

We now illustrate the performance of the method on a realistic problem by computing the development of a Rayleigh–Taylor instability in the viscous regime. This problem consists of two layers of fluid initially at rest in the rectangular domain $\Omega = (-d/2, d/2) \times (-2d, 2d)$. The initial density field is

$$\rho_0(x, y) = \rho_{\min}\big(2 + \tanh\big(\big(y - \eta(x)\big)/0.01d\big)\big), \quad \eta(x) = -0.1d\cos(2\pi x/d). \tag{18}$$

The heavy fluid is above and the density ratio is 3. For $t > 0$ the system evolves under the action of a vertical downward gravity field of intensity $\mathbf{g}$; the source term in the momentum equation is downward and equal to $\rho\mathbf{g}$.

The equations are non-dimensionalized using the following references: $\rho_{\min}$ for the density, d for lengths, and $d^{1/2}/g^{1/2}$ for time, where g is the gravity field. Then, the reference velocity is $d^{1/2}g^{1/2}$, and the Reynolds number is defined by $Re := \rho_{\min}d^{3/2}g^{1/2}/\mu$. The computational domain is restricted to $(0, d/2) \times (-2d, 2d)$ since we assume that the symmetry of the initial condition is maintained during the time evolution. The no-slip condition is enforced at the bottom and top walls and symmetry is imposed on the two vertical sides.

The mass conservation equation is stabilized by adding a non-linear viscosity proportional to the residual of the conservation equation for ρ^2 in the spirit of the entropy viscosity of [5].

The time evolution of the density field at $Re = 1000$ and $Re = 5000$ is shown in Fig. 1 at times $1/\sqrt{A_t}$, $1.5/\sqrt{A_t}$, $1.75/\sqrt{A_t}$, $2/\sqrt{A_t}$, $2.25/\sqrt{A_t}$, and $2.5/\sqrt{A_t}$ where $A_t = (\rho_{\max} - \rho_{\min})/(\rho_{\max} + \rho_{\min}) = 0.5$ is the Atwood number. The mesh is composed of 232 552 triangles and there are 466 573 $\mathbb{P}_2$ nodes. The mesh size is of order 0.025 in the refined regions. The time step is $\Delta t = 0.00125/\sqrt{A_t}$.

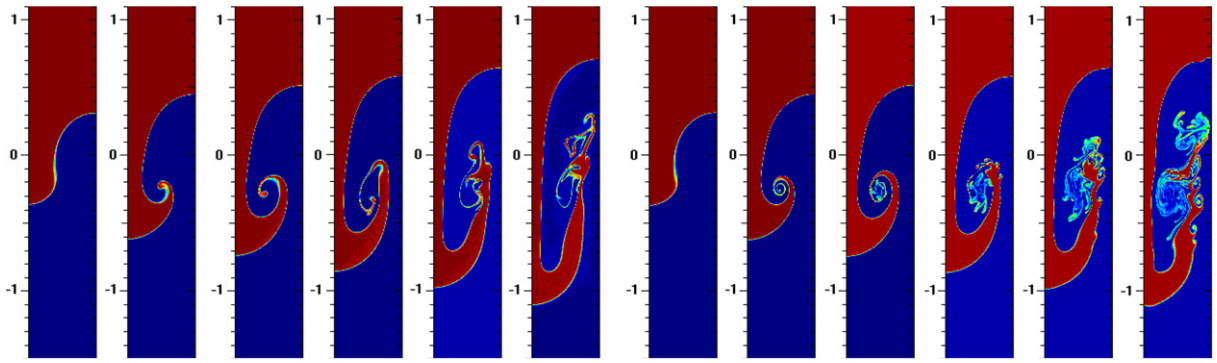

Fig. 1. The density field. $Re = 1000$ (left), $Re = 5000$ (right).

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