On the numerical simulation of the free fall problem

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Summary. The numerical simulation of the free fall of a solid body in a viscous fluid is a challenging task since it requires computational domains which usually need to be several order of magnitude larger than the solid body in order to avoid the influence of artificial boundaries. Toward an optimal mesh design in that context, we propose a method based on the *weighted* a posteriori error estimation of the finite element approximation of the fluid/body motion. A key ingredient for the proposed approach is the reformulation of the conservation and kinetic equations in the solid frame as well as the implicit treatment of the hydrodynamic forces and torque acting on the solid body in the weak formulation. Informations given by the solution of an adequate dual problem allow to control the discretization error of given functionals. The analysis encompasses the control of the the hydrodynamic force and torque on the body. Numerical experiments for the two dimensional sedimentation problem validate the method.

Key words: Finite element method, a posteriori error estimation, free steady fall problem, fluid-structure coupling

1 Introduction

Over the last decades, the study of the motion of small particles in viscous liquid has been the object of intensive research activities in fluid mechanics. The investigation topics range from the theoretical mathematical analysis (existence and uniqueness proof) (see e.g. [13, 5, 14] and references therein) to the numerical simulation of the liquid-particle interaction (see e.g. [6, 8, 11, 15] and references therein). The present paper concentrates on the numerical simulation of the steady free fall of a unique solid body in a viscous flow. Many aspects related to this problem are still not well understood. Especially, the issue of the stability of *terminal states* in dependency with the body geometry and orientation needs to be addressed. We propose in that context a new weighted a posteriori error estimator in order to control the discretization error and to design adequate mesh leading to economical discretization for computing the physical quantities of interest (see [1] and references therein). These features are of great importance since the numerical simulation of the free fall of a solid body in a viscous fluid requires computational domains which are usually several orders of magnitude larger than the solid body in order to avoid the influence of artificial boundaries.

The weighted a posteriori error estimator relies on the resolution of an adequate dual problem which gives localized sensitivity factors with regard to the error measured by means of given functional. The key ingredients of the error estimator derivations in our context are the reformulation of the conservation and kinetic equations in the solid body frame as well as the implicit treatment of the hydrodynamic forces and torque acting on the body in the weak formulation. Our analysis encompasses the control of the free fall velocity, the orientation of the body, the hydrodynamic force and torque on the body.

The outline of the remainder of this paper is as follows. In section 2, we briefly derive the formulation of the stationary free fall problem. Section 3 deals with the weak formulation of the equations of the fluid-body motion and its discretization by means of the finite element method. Section 4 is dedicated to the derivation of an a posteriori error estimator for the hydrodynamic force and torque acting on the solid body. In section 5, numerical experiments for the two dimensional sedimentation problem are presented to validate the method.

2 Problem formulation

2.1 General formulation of the fluid/body interaction

We consider the free fall of a solid body $\mathcal{S} \subset \mathbb{R}^d$ $(d = 2, 3)$ in an incompressible liquid $\mathcal{L}$ filling the whole space $\mathcal{D} := \mathbb{R}^d \backslash \mathcal{S}$. The solid body $\mathcal{S}$ is assumed to be a bounded domain and the velocity of its mass center C (resp. its angular velocity) is denoted by $\mathcal{V}_C$ (resp. Ω) in the inertial frame $\mathcal{F}$. The region occupied by $\mathcal{S}$ at time t is described by $S(t)$ and the corresponding attached frame is denoted by $\mathcal{R}(t)$. In the inertial frame $\mathcal{F}$ the equations of conservation of momentum and mass of $\mathcal{L}$ in their non conservative form are given by

$$\left.\begin{array}{c} \rho \frac{\partial \mathrm{v}}{\partial t} + \rho(\mathrm{v} \cdot \nabla)\mathrm{v} = \rho g + \nabla \cdot \mathcal{T}(\mathrm{v}, \mathrm{p}) \\ \nabla \cdot \mathrm{v} = 0 \end{array}\right\} \quad \text{for} \quad (x,t) \in \bigcup_{t>0} [\mathbb{R}^d \backslash S(t)] \times \{t\}, \qquad (1)$$

where ρ is the constant density of $\mathcal{L}$, v and p are the Eulerian velocity field and pressure associated with $\mathcal{L}$, $\mathcal{T}$ is the Cauchy stress tensor and ρg is the force of gravity which is assumed to be the only external force. We assume further a Navier-Stokes liquid model for which the Cauchy stress tensor is given by

$$\mathcal{T}(\mathrm{v},\mathrm{p}) := -\mathrm{p}\mathbf{1} + \mu(\nabla \mathrm{v} + (\nabla \mathrm{v})^T), \tag{2}$$

where μ is the shear viscosity. The boundary conditions are given by

$$\mathrm{v}(x,0) = 0, \qquad \lim_{|x|\to\infty} \mathrm{v}(x,t) = 0 \quad \text{for } x \in \mathbb{R}^d \backslash S(t) \tag{3}$$

$$\mathrm{v}(x,t) = \mathcal{V}_C(t) + \Omega(t) \times (x - x_C(t)) \ \text{ for } \ x \in \partial S(t). \tag{4}$$

The fluid/body coupling occurs through the Dirichlet boundary condition (4). It relies on the determination of the body motion which is obtained by requiring the balance of the linear and angular momentum:

$$\begin{cases} m_S \dot{\mathcal{V}}_C = m_S g - \displaystyle\int_{\partial S(t)} \mathcal{T}(\mathrm{v},\mathrm{p}) \cdot N \, d\sigma, \\ \frac{d(J_{S(t)} \cdot \Omega)}{dt} = - \displaystyle\int_{\partial S(t)} (x - x_C) \times [\mathcal{T}(\mathrm{v},\mathrm{p}) \cdot N] \, d\sigma, \end{cases} \tag{5}$$

where m_S is the mass of the body, N is the unit normal to $\partial S(t)$ oriented toward the body and J_S denotes the inertia tensor with respect to the mass center C. Further we assume $\mathcal{V}_C(0) = 0$, $\Omega(0) = 0$.

The straightforward formulation (1-5) has the disadvantage that the region occupied by the liquid $\mathcal{L}$ is time dependent. This can be avoided by reformulating these equations in the body frame $\mathcal{R}$(t). If y denotes the position of a point P in the frame $\mathcal{R}$(t) and x is the position of the same point in $\mathcal{F}$, we have

$$x = Q(t) \cdot y + x_C(t), \quad Q(0) = \mathbf{1}, \quad x_C(0) = 0, \tag{6}$$

with Q an orthogonal linear transformation. Considering the transformation (6) one can reformulate the system of equations (1) in the following form

$$\left.\begin{aligned} \rho\{\tfrac{\partial v}{\partial t} + ((v - V) \cdot \nabla) v + \omega \times v\} = \nabla \cdot T(v,p) + \rho G(t) \\ \nabla \cdot v = 0 \end{aligned}\right\} \tag{7}$$

for $(y,t) \in [\mathbb{R}^d \backslash S(0)] \times (0,\infty)$, where

$$v(y,t) := Q^T \cdot \mathrm{v}(Q \cdot y + x_C, t), \qquad p(y,t) := \mathrm{p}(Q \cdot y + x_C, t), \qquad G := Q^T \cdot g$$
$$V(y,t) := Q^T(\mathcal{V}_C + \Omega \times (Q \cdot y)), \quad T(v,p) := Q^T \cdot \mathcal{T}(Q \cdot v, p) \cdot Q, \quad \omega := Q^T \cdot \Omega.$$

The additional term $\omega \times v$ in the momentum equation $(7)_1$ corresponds to the *Coriolis force* induced by the frame transformation (6). Correspondingly the system equations (5) describing the motion of the body are transformed to

$$\begin{cases} m_S \dot{V}_C + m_S(\omega \times V_C) = m_S G(t) - \displaystyle\int_{\partial S} T(v,p) \cdot n \, d\sigma, \\ I_S \cdot \dot{\omega} + \omega \times (I_S \cdot \omega) = - \displaystyle\int_{\partial S} y \times [T(v,p) \cdot n] \, d\sigma, \\ \frac{dG}{dt} = G \times \omega, \end{cases} \tag{8}$$

where

$$V_C := Q^T \cdot \mathcal{V}_C, \quad n := Q^T \cdot N, \quad I_S := Q^T \cdot J_S \cdot Q, \quad \partial S := \partial S(0).$$

In order to keep compatible notations for both the two an three dimensional case, we assume for $d = 2$ that $\omega := (0, 0, \boldsymbol{\omega})$ and similarly $y \times [T \cdot n] = (0, 0, -y_2(T \cdot n)_1 + y_1(T \cdot n)_2)$. For $d = 2$, the equation $(8)_2$ reduces to a scalar equation.

In the body frame $\mathcal{R}$(t) the direction of the gravitational force G depends on the time t and becomes therefore an unknown to be resolved. The third additional equation of (8) provides the needed equation describing its variation. Its derivation relies on simple calculus related to the transformation (6). For more details regarding the overall derivation of these equations we refer to G.P. Galdi [5].

2.2 Formulation of the stationary free fall problem

The solid body $\mathcal{S}$ is said to undergo a *free steady fall* if the translational and angular velocity V_C and ω are constant and if the motion of the liquid $\mathcal{L}$ is stationary in the frame $\mathcal{R}(t)$. The study of such a configuration is of great interest since it corresponds to so called *terminate state* motions of sedimenting particles for which many questions still remain open: e.g. the number of possible terminal states for a given body geometry, the orientation of the solid body, the stability of the corresponding solution (see [5] and references therein). The free steady fall is thus obtained by requiring that v, p, V_C, ω and G are time independent. Comparing with (7-8), this leads to the following system of equations:

$$\left.\begin{array}{r} \rho\{((v - V) \cdot \nabla)v + \omega \times v\} = \nabla \cdot T(v, p) + \rho G \\ \nabla \cdot v = 0 \end{array}\right\} \quad \text{for} \quad y \in [\mathbb{R}^d \backslash S], \tag{9}$$

$$\lim_{|y| \to \infty} v(y) = 0 \tag{10}$$

$$v(y) = V(y) := V_C + \omega \times y \qquad \text{for} \quad y \in \partial S \tag{11}$$

$$m_S(\omega \times V_C) = m_s G - \int_{\partial S} T(v, p) \cdot n \; d\sigma, \tag{12}$$

$$\omega \times (I_S \cdot \omega) = -\int_{\partial S} y \times [T(v, p) \cdot n] \; d\sigma, \tag{13}$$

$$G \times \omega = 0. \tag{14}$$

The system of equations (9-14) describes different class of free fall regimes and configurations which are outlined in [9]. They lead to different problem formulations. For the most general setup, we assume $\omega \neq 0$. Due to equation (14), this configuration can be attained only for $d = 3$. Further it imposes G parallel to ω. The free steady fall problem can then be stated as

Problem 1. Assume $d = 3$. Given ρ, $T = T(v, p)$, $|G| = |g|$, I_S and m_S, find v, p, V_C, ω, G whereas $G = |g||\omega|^{-1}\omega$ if $\omega \neq 0$, such that (9-13) holds.

3 Galerkin finite element discretization

For a domain $\Omega \subset \mathbb{R}^d$, let $L^2(\Omega)$ denote the Lebesgue space of square-integrable functions on Ω equipped with the inner product and norm

$$(f, g)_\Omega := \int_\Omega fg \; dx, \qquad ||f||_\Omega := (\int_\Omega |f|^2 \; dx)^{\frac{1}{2}}.$$

Analogously, $L^2(\partial\Omega)$ denotes the space of square integrable functions defined on the boundary $\partial\Omega$. The L^2 functions with generalized (in the sense of distributions) first-order derivatives in $L^2(\Omega)$ form the Sobolev space H^1, while $H^1_0 = \{v \in H^1(\Omega), v|_{\partial\Omega} = 0\}$.

3.1 Variational formulation

The Galerkin finite element method starts from a variational formulation of the equations to be solved. We first consider the most general setup of problem 1 i.e. $\omega \neq 0$ and the related equations (9-13). The key ingredient for the derivation of a weak form of the equations (9-13) is an adequate choice of the velocity space allowing to eliminate the explicit formulation of the hydrodynamic force and torque on the solid body needed for the kinematic equations (12) and (13). This can be obtained by including the no-slip Dirichlet condition (11) in the velocity space:

$$\mathcal{H}_1(D) := \left\{(v, V, \omega) : \; v \in [H^1_{loc}(\overline{D})]^d, V \in \mathbb{R}^d, \; \omega \in \mathbb{R}^d, v = V + \omega \times y \text{ on } \partial S\right\}, \tag{15}$$

where $D := \mathbb{R}^d \backslash S$. The pressure p which is defined modulo constants is assumed to lie in the space

$$L^2_0(D) := \left\{ q \in L^2(D) : \; \int_{D'} q = 0 \right\}. \tag{16}$$

where $D' \subset D$ bounded. For $u := \{(v, V_C, \omega), p\} \in \mathcal{H}_1(D) \times L^2_0(D)$ and $\phi := \{(\varphi, \phi_1, \phi_2), q\} \in \mathcal{H}_1(D) \times L^2_0(D)$ we define the following semi-linear form

$$\begin{aligned}\mathcal{A}_1(u; \phi) := \rho(((v - (V_C + \omega \times y)) \cdot \nabla)v, \varphi)_D + (\omega \times v, \varphi)_D \\ -(p, \nabla \cdot \varphi)_D + 2\mu \int_D D(v) : D(\varphi) - (\rho|g||\omega|^{-1}\omega, \varphi)_D \\ -\phi_1 \cdot [m_S(|g||\omega|^{-1}\omega - \omega \times V_C)] + \phi_2 \cdot [\omega \times (I_S \cdot \omega)] \\ -(\nabla \cdot v, q)_D,\end{aligned} \tag{17}$$

which is obtained by testing the equations (9) and (12-13) by $\phi \in \mathcal{H}_1(D) \times L_0^2(D)$ and by integration by parts of the diffusive terms and the pressure gradient in $(9)_1$. $D(v)$ denotes the deformation tensor i.e. $D(v) := \frac{1}{2}(\nabla v + (\nabla v)^T)$. A weak form of problem 1 can therefore be formulated as

Problem V1. Find $u := \{(v, V_C, \omega), p\} \in \mathcal{H}_1(D) \times L_0^2(D)$ such that

$$\mathcal{A}_1(u; \phi) = 0 \quad \forall \phi \in \mathcal{H}_1(D) \times L_0^2(D). \tag{18}$$

The equation modeling the balance of the linear (resp. angular) momentum (12) (resp. (13)) can obviously be recovered by testing in (18) with the functions $\{(0, \phi_1, 0), 0\}$ (resp. $\{(0, 0, \phi_2), 0\}$).

Remark 1. The advantages of the formulation (18) rely on the fact that the force and torque on the solid body do not need to be computed explicitly. Numerical instabilities arising for the computation of these lower dimensional integrals can therefore be avoided (see [7, 12]).

3.2 Finite element discretization

First of all, the unbounded domain $D := \mathbb{R}^d \backslash S$ filled by the liquid $\mathcal{L}$ is replaced by a bounded domain $\Omega \subset \mathbb{R}^d \backslash S$. On the artificial boundary $\partial\Omega \backslash \partial S$ we prescribe homogeneous Dirichlet boundary conditions,

$$v(y) = 0 \qquad \text{for } y \in \partial\Omega \backslash \partial S.$$

In order to ensure that the impact of this simplification on the quantities of interest is smaller than the discretization error, we have to chose Ω large enough. For a detailed discussion of this issue we refer to [2, 16].

The discretization uses a conforming finite element space $W_1^h \subset \mathcal{H}_1(\Omega) \times L_0^2(\Omega)$ defined on a triangulation $\mathcal{T}_h = \{K\}$ consisting of quadrilateral or hexahedral cells K covering the domain $\overline{\Omega}$; the family of triangulations $\{\mathcal{T}_h\}_h$ is assumed to be quasi-uniform as $h \to 0$. For the trial and test spaces $W_1^h \subset \mathcal{H}_1(\Omega) \times L_0^2(\Omega)$ we consider the standard Hood-Taylor finite element [10] i.e.

$$\begin{aligned} W_1^h := \big\{ ((v, V, \omega), p) \in \big\{ [C(\overline{\Omega})]^d \times \mathbb{R}^d \times \mathbb{R}^d \big\} \times C(\overline{\Omega}), \\ v|_K \in [Q_2]^d, p|_K \in Q_1, v|_{\partial S} = V + \omega \times y \big\}, \end{aligned}$$

where Q_r describes the space of isoparametric tensor-product polynomials of degree r (for a detailed description of this standard construction process see e.g. [3]). This choice for the trial and test functions has the advantage that it guarantees a stable approximation of the pressure since the uniform *Babuska-Brezzi* inf-sup stability condition is satisfied uniformly (see [4] and references therein). Compared to equal order function spaces for the pressure and the velocity, no additional stabilization terms are needed. Further, in order to facilitate local mesh refinement and coarsening, we allow the cells in the refinement zone to have nodes which lie on faces of neighboring cells (see figure 1). The degrees of freedom corresponding to such hanging nodes are eliminated by interpolation enforcing global conformity for the finite element functions. The discrete counterpart of problem (V1) reads

Problem $V1'$**.** Find $u_h := W_1^h$ such that

$$\mathcal{A}_1(u_h;\phi_h) = 0 \quad \forall \phi_h \in W_1^h. \tag{19}$$

4 A posteriori error control for the hydrodynamical force and torque

The implicit treatment of the hydrodynamical force and torque acting on the solid body $\mathcal{S}$ in terms of the natural boundary conditions (see section 3.1) allows to derive a specific a posteriori error control strategy. The proposed approach, inspired by the work of Giles et al. [7], takes great advantage of the special structure of the free steady fall problem and of the considered weak formulation leading to a natural derivation of error bounds for the hydrodynamical force and torque.
We consider the most general setup of problem 1 and define for $u := \{(v, V_C, \omega), p\} \in \mathcal{H}_1(D) \times L_0^2(D)$ the following weighted functional

$$J_\psi(u) := \int_{\partial S} [T(v,p)\cdot n]\cdot \psi \; d\sigma, \tag{20}$$

where $\psi := \psi_1 + \psi_2 \times y \in \mathbb{R}^3$ with $\psi_1, \psi_2 \in \mathbb{R}^3$. For $\psi = \psi_1$ (resp. $\psi = \psi_2 \times y$), the functional $J_\psi(u)$ corresponds obviously to the weighted hydrodynamical force (resp. hydrodynamical torque) since

$$J_{\psi_1}(u) = \psi_1 \cdot \int_{\partial S} [T(v,p)\cdot n] \; d\sigma \tag{21}$$

$$J_{\psi_2\times y}(u) = \psi_2 \cdot \int_{\partial S} y \times [T(v,p)\cdot n] \; d\sigma. \tag{22}$$

Now, we define the following semi-linear form

$$\begin{aligned} \mathcal{A}(u;\phi) := \rho(((v-(V_C+\omega\times y))\cdot\nabla)v,\varphi)_D + (\omega\times v,\varphi)_D \\ -(p,\nabla\cdot\varphi)_D + 2\mu\int_D D(v):D(\varphi) \\ -(\rho|g||\omega|^{-1}\omega,\varphi)_D - (\nabla\cdot v, q)_D, \end{aligned} \tag{23}$$

which, apart from the boundary terms ϕ_1 and ϕ_2, corresponds to the semi-linear form $\mathcal{A}_1(u;\phi)$. Further we define the following velocity space

$$\mathcal{H}_1^\psi(D) := \mathcal{H}_1(D) \cap \{(v,V,\omega) : \; \nabla\cdot v = 0 \;\text{ in }\; \Omega, \; V=\psi_1, \; \omega=\psi_2\}. \tag{24}$$

Then following lemma holds (see [9]):

Lemma 1. *Under sufficient regularity assumptions for the solution u of problem V1, we have*

$$J_\psi(u) = \mathcal{A}(u; w) \quad \forall w \in \mathcal{H}_1^\psi(D) \times L_0^2(D). \tag{25}$$

The discrete counterpart of $\mathcal{H}_1^\psi(D) \times L_0^2(D)$ is defined as

$$W_1^{\psi,h} := W_1^h \cap \{((v, V, \omega), p) : \; V = \psi_1, \; \omega = \psi_2\}.$$

Let $u_h \in W_1^h$ be the solution of the discrete problem $V1'$. One can easily show that the functional

$$\tilde{J}_\psi(u_h) := \mathcal{A}(u_h; w) \quad \forall w \in W_1^{\psi,h}, \tag{26}$$

is well defined since $\mathcal{A}(u_h; w)$ depends uniquely on the boundary value ψ of w. It is of importance to notice that in general

$$\tilde{J}_\psi(u_h) \neq J_\psi(u_h).$$

As shown in [7], the functional $\tilde{J}_\psi(u_h)$, rather than $J_\psi(u_h)$ is the appropriate approximation of $J_\psi(u)$. From now on, our purpose is then to derive error bounds for $J_\psi(u_h) - \tilde{J}_\psi(u_h)$. In order to derive an error representation for the error $J_\psi(u_h) - \tilde{J}_\psi(u_h)$, we define the following *linearized dual problem*:

Problem 4. Find $z := \{(z^v, z^{V_C}, z^\omega), z^p\} \in \mathcal{H}_1^\psi(D) \times L_0^2(D)$ such that

$$L(u, u_h; z, \phi) = 0 \quad \forall \phi \in \mathcal{H}_1^{\psi=0}(D) \times L_0^2(D). \tag{27}$$

Here, $L(u, u_h; z, \phi)$ is assumed to be a bilinear form in z and ϕ chosen such that the following equality holds

$$L(u, u_h; z, u - u_h) = \mathcal{A}(u; z) - \mathcal{A}(u_h, z) \quad \forall z \in \mathcal{H}_1(D) \times L_0^2(D), \tag{28}$$

where u (resp. u_h) describes the solution of problem V1 (resp. $V1'$).
Due to the special nature of the nonlinear terms in $\mathcal{A}(\cdot; \cdot)$, $L(u, u_h; \cdot, \cdot)$ can be defined explicitly (see [9] for more details). Using these preliminaries we are now able to derive the needed error representation of $J_\psi(u_h) - \tilde{J}_\psi(u_h)$.

Proposition 1. *Let z be the solution of problem 4. Further let $\Pi : \mathcal{H}_1^\psi(D) \times L_0^2(D) \to W_1^{\psi,h}$ be some interpolation operator. We then have*

$$J_\psi(u_h) - \tilde{J}_\psi(u_h) = \mathcal{A}(u_h, z - \Pi z). \tag{29}$$

Proof. See [9].

Remark 2. The error representation (29) allows not only to control separately the hydrodynamical force and torque but also a weighted combination of both quantities. This can be done by an adequate definition of the weights ψ_1 and ψ_2 of the trace $\psi = \psi_1 + \psi_2 \times y$ in (25) and (26), respectively. The dual solution z depends on ψ exclusively through the enforcement of the Dirichlet boundary condition $z^v|_{\partial S} = \psi$.

5 Numerical experiments

We consider the free fall of a rectangular body of length $l = 6.10^{-2}m$ and width $L = 1.10^{-2}$ in a viscous fluid. The shear viscosity (resp. the density) is assumed to be $\mu = 0.1$ (resp. $\rho = 1$). Our numerical simulations lead to both horizontal and vertical position as terminal state. The vertical fall is however an instable terminal state and will not be further considered in the following (see figure 1). We assume homogeneous Dirichlet boundary conditions for the velocity on the outer boundary $\partial\Omega\backslash\partial S$ of the computational domain Ω (see [2] for more details). The large size needed for the computational domains imposes a careful mesh design. The a posteriori error estimates developed in section 4 allow to tackle this problem since it allows to construct economical meshes oriented toward the computation of a given parameter. Adaptive grids based on the a posteriori estimator (29) are plotted in figure 1.

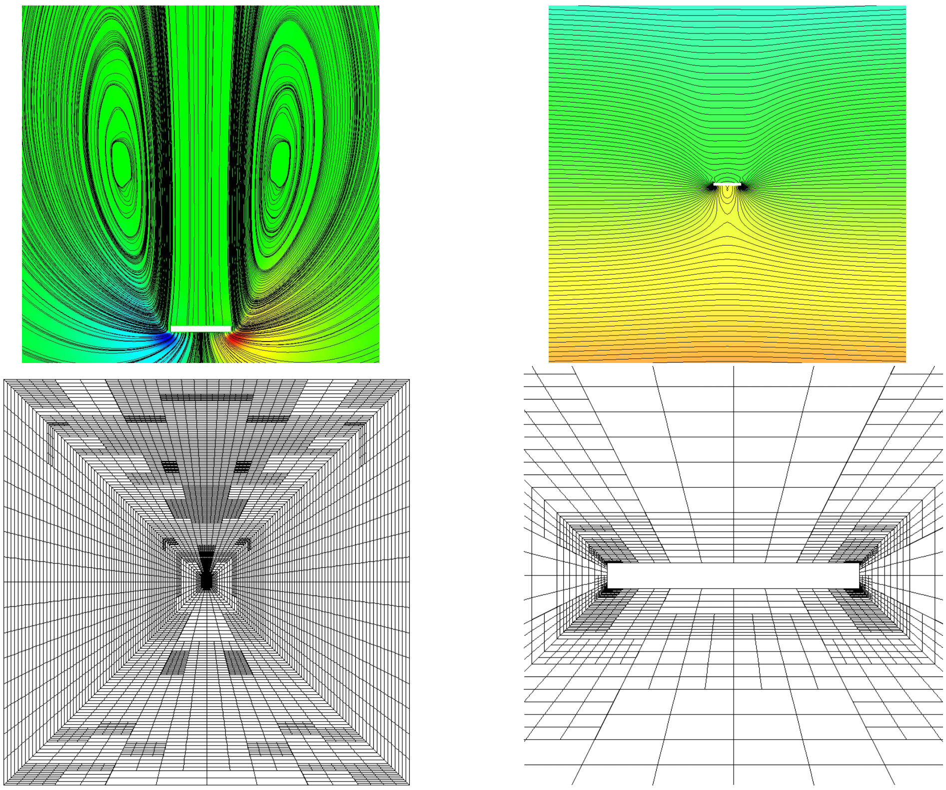

Fig. 1. (top left) Streamlines around the falling body for $\nu = 0.1$; (top right) pressure isolines; (bottom left and right) adaptive mesh obtains by means of (29) on a domain with diameter $D = 800$ and corresponding zoom around the body

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