Design and Construction of Computer Experiments in Fluid Mechanics and Ship Stability

Alexander Degtyarev*, Vasily Khramushin and Vladimir Mareev

Dept. of Computer Modelling and Multiprocessor Systems, Faculty of Applied Mathematics and Control Processes, St.Petersburg State University, Russia

Abstract: The paper considers a generalized functional and algorithmic construction of direct computational experiments in fluid dynamics. Tensor mathematics naturally embedded in the finite- operation in the construction of numerical schemes. As an elementary computing object large fluid particle which has a finite size, its own weight, internal displacement and deformation is considered. The proposed approach focuses on the use of explicit numerical schemes. The numerical solution of the problem is divided into several stages that are a combination of Lagrange and Euler methods.

Key words: Fluid mechanics, direct computational experiment, computational efficiency

1. Introduction

In the paper mathematical basis for direct computational hydroaeromechanic experiment formation is considered. In contrast to the traditional approach of finite difference numerical schemes construction that are output from analytical models in the form of partial differential equations [1], the proposed techniques are focused on the construction and use of direct computational experiments. For these purposes fundamental laws of motion [2] are applied to large fluid particles [3], which have a finite size, their own weight, internal displacement and deformation [4, 5]. Each particle is represented in world (global) and local coordinate systems [6, 7]. It gives opportunity to examine them as free particles with strictly defined laws of neighbor interaction and with alternation of modeling stages of independent internal transformation processes [8, 9]. Such modeling is carried out in accordance with the basic conservation laws of energy, mass and fluid continuity [10, 11]. With this approach mathematical description of physical processes in aerohydrodynamics is greatly enhanced. It is the better than the traditional mathematical models based on differential calculus of infinitesimal elements [12], which basically do not allow direct control of internal state of measurable fluid volumes. At the same time the proposed approach differs from the well known smooth particle hydrodynamics (SPH) simulation [13-16], which is a purely Lagrangian method. For better numerical realization we combine Lagrangian and Eulear approaches at different stages.

Strict and mutually reversible mathematical definition of properties and description of mechanics of finite fluid volumes transformations are possible using classical tools of tensor calculus. This instrument sufficiently specifies transformation of complex fluid flows through first-order spatial approximations.

It is shown in the paper that with the proposed approach hydromechanics problems can be reduced to the use of explicit numerical schemes. At the same time tensor form of state control of three-dimensional computational objects and processes allows to tailor the solution to the real laws of motion or to the empirical and the asymptotic dependences. Apparatus of three-dimensional tensor mathematics in a natural way is embedded in the finite-difference operations of

large particles (final volume) method. This is done in a strict and an unambiguous representation of the physical laws in the nearest vicinity of an elementary particle continuum. In the paper carrying out of numerical experiments in a natural way comes down to three conditionally independent physical processes. This fact, combined with predominant use of explicit numerical schemes, enables natural parallel computing with the ability to dynamically select appropriate hydrodynamics laws. This choice is carried out depending on the characteristics of transformation and interaction of considered computational objects (particles).

In practice, the constructions of direct computational experiments are usually obtained from close analogs of the numerical schemes from systems of partial differential equations. However, these analogs differ as short canonical result expressions in the final difference form [17]. For them, the results of the calculations are more appropriate for comparisons with physical or full scale experiments than for analytically accurate but simplistic solutions of classical mathematical physics.

It should be noted that the above considerations are not new or unexpected. This work is focused on overcoming of two "eternal" questions in computational fluid mechanics:

1. incomplete adequacy of the Navier-Stokes equations;
2. problems arising in discretization of the equation.

The essence of the first question is that the Navier-Stokes equation is not closed [19]. Therefore at the solution of these equations in different cases various closing ratios are put into practice [1, 22]. These ratios have character of conservation laws. Thus, the first problem of hydrodynamics is isolation of physical model of considered system from the actual situation.

The problems arising at discretization of the model equations of hydrodynamics, are also quite serious. Firstly, equation change-type at its finite-difference representation is possible [22, 23]. Secondly, the hydrodynamic nature of the studied phenomena is far from concept of infinitesimals with which we work at consideration of any differential equations [12, 17]. In contrast to the problems of strength and elasticity of solid body, where deflections, shifts, turns may be considered in the finite-difference representation as smalls, shift of particles in continuous medium hydrodynamic problems even with a small impact may be finite.

Thus, as a result we not only have fundamentally wrong equation as a model, but we often incorrectly numerically solve it. Therefore our task, in essence, consists in tearing off calculations from representation of model of physical system. For the solution of this problem methods of the direct computing experiment based on the modern computer architecture are developed in the paper.

2. Numerical construction of continuous medium objects

Direct numerical experiments in continuum mechanics using digital discrete computers are based on a limited set of numeric objects which interpolate parameters of the state of the physical fields in time. Computational processes with such numerical objects have to take place in accordance with physical laws in the mesh areas (including nonregularized ones). At the same time each mesh cell is represented as independent corpuscle actively interacting with the surrounding cell particles [12].

Let us call one mesh cell as elementary computational object (large particle of continuous medium of finite volume). All internal transformation of such particle within linear approximations is strictly and uniquely determined by the rules of tensor arithmetics. This is a convenient tool for geometric and kinematic description of a large particle. Apart from its position in space, classical tensor calculus

describes more complex transformation: rotation, compression, elastic deformation etc. Its functional apparatus is sufficient for development of strong forward and reverse mathematical description of physical processes of fluid mechanics in the finite mesh area.

For description of large mobile elementary particles in a three-dimensional space we introduce two coordinate systems: absolute and mobile local (associated with the particle) (Fig. 1).

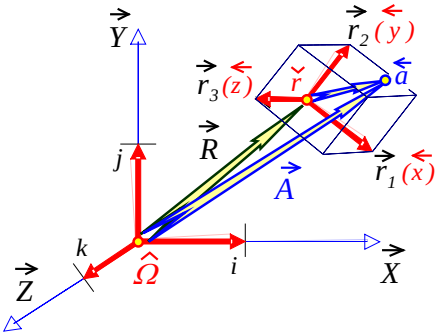

Fig. 1 – Local basis r_i is formed by triad of basis vectors, ijk – unit vectors of global coordinate system (XYZ); *R* – radius vector of the moving system; *A* - radius vector of the point in global coordinate system; $\breve{a}$ - the same point in local coordinate system

Let us initially restrict our consideration of distant mechanical interference. Then mechanical laws for local interaction set big external force interactions, intensive inertial reactions and sufficient internal deformations. All laws of fluid kinematics and mechanics of its transformation are represented as linear spatio-temporal dependencies in the simplest tensor-vector form.

Let us distinguish the following notations of vector and tensor quantities for the convenience of representation of analytic expressions in their direct relationship with finite-difference representations and earlier restrictions [12]:

A – value measured in a global coordinate system (may be scalar or vector only)

a – value measured in a local basis, it refers to small volume or contiguous particles only (differential differences, can be scalar, vector or tensor)

$\vec{R},\vec{r}$ – values projected on global basis

$\breve{R},\breve{r}$ – values projected on local basis

$\hat{r}$ – local tensor in projections of global system

$\breve{r}$ – local tensor in projections of local system

Detailed notation is in appendix 1.

With this alphabet, capital letters for values in global coordinate system are used. Lower letters are used for small quantities at local bases projections in spatial location and current time. Basic mathematical operations are tensors products and products of tensors and vectors. They define the ratio of local reactions of the fluid particles to external influences of the environment. Formally possibility of rank increasing of tensor-vector objects is excluded. They have not immediate physical interpretation.

Absolute or full velocity vector of a large particle is introduced as a shift of the center of mass in the global coordinate system:

$$\vec{V}\cdot t = {}^{\Delta}\vec{R} = {}^{t}\vec{R} - {}^{0}\vec{R} = {}^{T-t}\vec{R} - {}^{T}\vec{R} \qquad (1)$$

Tensor of instantaneous velocities relative to the conditional center of large particle in projections on absolute coordinate system is assembled by direct geometric constructions. Obviously, such tensor contains components of rotation and speed of mutual deformation of the basis vectors for the adjacent dots in the fluid flow:

$$\hat{\omega} = \vec{\omega}^{i} = {}_{\Delta}\vec{V}_i = {}_{+}\vec{V}_i - {}_{\Omega}\vec{V}_i \qquad (2)$$

At the initial moment tensor internal flow velocities equal to zero. This is acceptable on the Euler stages of computational experiment.

Kinematics of internal flows in elementary fluid particle is also algorithmically constructed as differential velocity tensor (Fig. 2).

This is tensor of basis vectors form of large fluid particle moveable in time:

$$\hat{v}\cdot t = \vec{v}_i \cdot t = {}^{\Delta}_{\Delta}\vec{r}_i = {}^{t}_{+}\vec{r}_i - {}^{o}_{\Omega}\vec{r}_i \quad [m^3] \qquad (3)$$

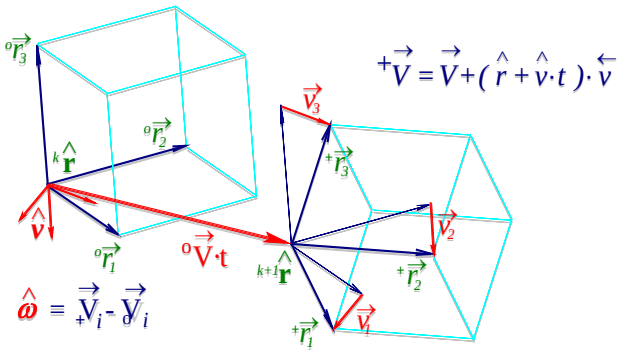

Fig. 2 – Tensor of local velocities is formed by deformation displacements of basis vectors of large fluid particle for rated time interval

Tensor $\hat{v}$ sets current speed of the unit vectors in the local basis (lower case) with respect to the global coordinate system (subscripts). For traditional analysis it can be transferred to the local reference system (normalization of geometric measurements):

$$\hat{v} = \hat{v} \cdot \hat{r} = \hat{v} / \hat{r} \quad [s^{-1}] \qquad (4)$$

Here the known tensor of convective velocities is automatically formed. Traditional definition of an affinor is applicable to it and the theorem of Helmholtz [4] for decomposition on small increments in time is fair: expansion (divergence); turn (rotor) and deformation (shift).

3. Definition of space operations over the elementary particles of fluid

Computing objects are created at a stage of initial formation of hydrodynamic fields in the form of mesh area. The mesh area is supposed dynamically changeable and the irregular depending on current regimes in local areas and features of the problem. These objects are under construction immediately during computing experiment. Their appearance is the result of special logical procedures that control specific regimes of fluid flow and control progress of computational experiment on a functional level. A striking example of such procedure is the change of mesh area in zones of cavitation and vortex breaks and also on the free surfaces. Computing objects cannot be generated or destroyed as a result of mathematical manipulations (generation of vector dyads or tensors of the third rank are excluded by logic of creation of computing objects) [17].

Control of physical state of considered objects (large particles) allows to choose type of computing operations dynamically. For correct carrying out direct computing experiment it is necessary to set the following requirements to mathematical models:

1. Elementary spatio-temporal objects and the basic physical phenomena must be described in the dimensional form;
2. Physical properties of the environment and mechanics laws for the modelled phenomena are formulated in canonical form. Transition to demanded reference systems is carried out automatically at algorithmic level.
3. Properties of arithmetic operations and elementary numerical objects are invariantly defined in global coordinate system and definitely correspond to calculated values in local bases. It is carried out by multiplication operations

Taking into account the history of the movement, "not free" fluid particle is governed by vector analog of the Newton law [5] (fig.3)

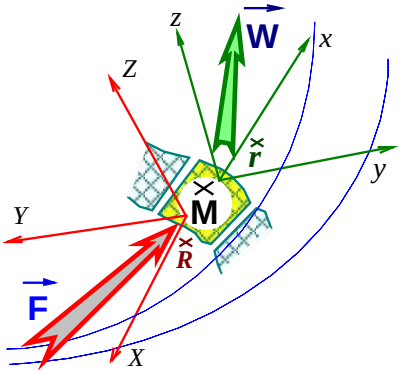

Fig. 1.

$$W_i = F_j \cdot M^{j}{}_{i} \quad \text{or} \quad \vec{W} = \vec{F} \cdot \overset{<}{M}, \qquad (5)$$

where external force $\vec{F}$ affects the large fluid particle allocated from stream $\overset{>}{M}$ and causes

reaction $\vec{W}$. $\times$ icon above the letters in fig.3 means that it can be both $\wedge$ and $\vee$. Value and direction of $\vec{W}$ depend both on internal state (inertia) of this particle, and on its ability to be deformed, to absorb or to strengthen external manifestations of motion energy. Linking mass tensor with the fluid particles $\overset{>}{M} = \hat{r} \cdot \check{\rho}$ we obtain the definition of density or internal energy, which imparts fluid environment anisotropic properties:

$$\vec{F} = r_{ik} \cdot \rho^{kj} \cdot \vec{W} = \hat{r} \cdot \check{\rho} \cdot \vec{W}, \qquad (6)$$

where $\hat{r}$ [m^3] is tensor of large fluid particle form; $\check{\rho}$ [kg/m^3] is density tensor characterizing the internal state of a fluid particle, taking into account the dynamic interaction with the continuous medium.

Small spatial movements historically are determined by the calculus of fluxions underlying Newtonian mechanics. In kinematic problem fluxions determine the speed forming difference differential (by Newton – the moment) in a product with calculated step in time.

Within such views large particle kinematics is given by differential (moment) of velocities in the absolute coordinate system subject to small displacements in the local basis:

$$^{+}\vec{A} = \vec{R} + \vec{V} \cdot t + \vec{Z}, \qquad (7)$$

where t is calculated time moment; $\overleftarrow{a}$ is coordinates of the control point (see fig.1) in local reference system; $\vec{R}$ is location of the local basis in the absolute coordinate system; $\vec{V}$ is speed of forward shift of local basis (of large fluid particle); $\vec{Z}$ may be in different form in dependence of mode of current. In simplest case $\vec{Z} = \overleftarrow{a} \cdot (\hat{r} + \hat{v} \cdot t)$. Then we represent (7) as $^{+}\vec{A} = {}^{0}\vec{A} + (\vec{V} + \overleftarrow{a} \cdot \hat{v}) \cdot t$ or in the form of system of scalar equations [6]:

$$^{+}A_x = {}^{o}A_x + \left(V_x + a^x v_{xx} + a^y v_{yx} + a^z v_{zx}\right);$$
$$^{+}A_y = {}^{o}A_y + \left(V_y + a^x v_{xy} + a^y v_{yy} + a^z v_{zy}\right);$$
$$^{+}A_z = {}^{o}A_z + \left(V_z + a^x v_{xz} + a^y v_{yz} + a^z v_{zz}\right).$$

In case of vortex flow in accordance with Cauchy-Helmholtz theorem [4] $^{+}\vec{A} = \vec{R} + \vec{V} \cdot t + \overleftarrow{a} \cdot (\hat{r} + \hat{v} \cdot t) + \overleftarrow{\omega} \cdot (\hat{r} + \hat{v} \cdot t) \cdot t$. Here $^{+}\vec{A}$ and $^{0}\vec{A}$ are new and initial location of control point in global system; $\hat{r}$ is tensor of large fluid particle form; $\hat{v}$ is tensor of speeds of local motions of basic axes of the tensor defining deformation of a large fluid particle; $\overleftarrow{\omega}$ is speed of internal shift.

Let us present equation for motion of arbitrary point (7) near large fluid particle in convenient dynamic form. Here we take into account deformation and energy of internal forces: $\overset{>}{m}$ [kg^{-1}]. We have to consider multiple nature of such forces: external distributed $\hat{f}$ [*N m^2, kg m^3/s^2*] and mass $\vec{F}$ [*N, kg m/s^2*]:

$$^{+}\vec{A} = \vec{R} + \vec{V} \cdot t + \overset{>}{m} \cdot \vec{F} \cdot t^2/2 + (\hat{r} + \hat{v} \cdot t + \overset{>}{m} \cdot \hat{f} \cdot t^2/2) \cdot \overleftarrow{a}, \qquad (8)$$

The resulting expression contains the traditional system of Euler differential equations and an additional term describing the deformation of a large fluid particle under the influence of stress on its borders.

4. Algorithmic realization of hydrodynamic laws

The Algorithmic implementation is based on computational schemes of mixed Lagrangian and Eulerian approaches [4,5]. This is expressed similar to the methods of "large particles" [3] and "final volume" [18] in the double integration of first order motion equations. Thus the time cycle of computing experiment is divided into three conditional stages:

1 stage – Kinematic parameters are calculated for the centers of large fluid particles. For this purpose, the current source data into fixed nodes of Eulerian coordinates are used;

2 stage – Lagrangian or large deformable fluid particles are involved in free motion. They redistribute the internal properties of the original Euler cells to adjacent space;

3 stage – Laws of conservation of mass and energy are consistent. This is achieved by deformation of

shifted fluid particles. The next step makes reinterpolation of characteristics of current in initial nodes of the fixed Euler computational mesh.

Computational experiment is generally presented as a process of integral transformation of the velocity field in absolute time:

$$^{+}\vec{V} = \vec{V} + \vec{W} \cdot t \,, \tag{9}$$

Thus the construction of computational experiment is reduced to difference derivation of the first order. This is the main feature of the Lagrangian-Eulerian approach for the numerical solution of problems in fluid mechanics. In other words, it is possible to call this approach a method of splitting of the decision on physical processes, which can be formed by three conditional stages of the numerical solution of applied problem:

1 stage. Basing on the current velocity field the condition of large fluid particles on the following instant is specified:

$$^{+}\overset{<}{M} = \overset{\vee}{\rho} \cdot (\hat{r} + \hat{v} \cdot t) \,, \tag{10}$$

where $\hat{v}$ is tensor of map of the current velocity field on local basis of a large particle; $\overset{\vee}{\rho}$ is tensor of internal state of a fluid particle at the current time moment.

2 stage. After specification of resultant vector of all external forces influencing a large fluid particle, calculation of new velocity field is carried out:

$$^{+}\vec{V} = \vec{V} + \overset{<}{M}^{-1} \cdot \vec{F} \cdot t \,, \tag{11}$$

3 stage. As a result of the first two phases spatial displacement of large fluid particles takes place. New hydrodynamic fields partly no longer satisfy the conditions of continuity and isotropic of source environment. Depending on task the type of problem, at the final stage it is necessary to make relaxational amendments to absolute properties and interaction conditions between fluid particles. It is necessary to carry out walkthrough control of quality of the solution. We must, if necessary, apply scheme of adaptation or empirical substitution of solution in areas where the computational model gives a clearly incorrect results.

It is known that traditional approach to numerical solution fluid dynamics problems is most often reduced to application of implicit schemes [1, 10]. The described algorithmic approach, first of all because of the proposed splitting of the solution on physical processes, gives the chance of application explicit numerical schemes at the first two stages. In this case it is possible to increase essentially effectiveness of computing procedures through:

1. Natural parallelization of the computation process;
2. Possibilities of adaptive correction of mesh area depending on features of the problem;
3. Dynamic reconstruction of solution in accordance with fluid currents transformations in time.

5. Construction of explicit numerical schemes and features of computational operations

Let us construct numerical procedure basing on the made assumptions. It is necessary to note that proposed approach (first of all endows the elementary deformable particle with internal energy) expands possibilities of mathematical representation of fundamental mechanics laws.

1. Vector analog of Newton law for deformable particle – equation (6).
2. Viscous stress tensor for Newtonian fluids:
$$\overset{>}{f}_{н} = \hat{v}_{н} \cdot \overset{\vee}{\eta} / \Lambda = \overset{>}{v}_{н} \cdot \eta / \Lambda \,, \quad [N/m] \tag{12}$$
3. Elastic stress tensor for a solid (Hooke law):
$$\overset{>}{f}_{\Gamma} = (\hat{r} + \hat{v}_{\Gamma} \cdot t) \cdot \overset{\vee}{c} / \Lambda \quad = (\overset{\times}{1} + \overset{>}{v}_{\Gamma} \cdot t) \cdot \overset{>}{c} / \Lambda \,, [N/m] \tag{13}$$

where tensor of local velocities is constructed as $\hat{v} = {}_{+}\vec{V}_i - {}_{o}\vec{V}_i$ (fig.2); general rheological constants are formally constructed in tensor form, they satisfy the expressions of the type $\overset{<}{M} = M^{i}_{k} = \overset{\vee}{\rho} \cdot \hat{r} = \rho^{ij} \cdot r_{jk}$ – tensor of inertia in projection on global reference system; $\hat{r}$, $\overset{\vee}{\rho}$ – geometric tensor of form [m^3] and fluid density [kg/m^3] and energy accumulation inside

the particle; $\overset{>}{\eta},\overset{>}{c}$ – tensors of dynamic viscosity [kg/s] and rigidity [kg] of real fluid; Λ – conditional distance that defines distance of upstream direction of adjacent particles.

5.1 Properties of computational operations

For correct construction of numerical schemes it is necessary to define properties of computational operation basing on proposed approach. All operations are carried out exclusively in the dimensional form. It is necessary to provide automatic control of the physical correctness of the simulated processes. If necessary hybrid schemes in subareas where there is a change of modes of the currents demanding well-timed substitution of used laws of mechanics and their mathematical models are applied. Three groups of operations contact computing objects:

1. Logical and empirical operations. There are physical laws like "if we have tensor of convective velocities $\overset{>}{v}$ then it generates tensor of stress $\overset{\vee}{f}$ in accordance with law (12)", etc. Such operations set a way of formation and methods of analysis of tensor objects, and also a decision making about change of mathematical models during calculations.
2. Addition operations are applied only to values with identical physical dimensions. Thus the condition of their definition and construction in the same basis has to be satisfied. Addition can be applied to the complex objects also in conditions when operations of automatic coordination of reference systems and physical dimensions are defined.
3. The operation "multiplication" is applicable only to objects whose connected components lie in dual systems of references. Increase of rank of tensor in multiplication operations is forbidden. For creation of vector or tensor objects special algorithms basing on a physical problem definition have to be defined.

Computational objects are given by the following characteristics:

1. Scalar and invariant values (time for example) take part just only in multiplication operations with any objects;
2. Vector values take part in addition operations with comparable vectors, they can take part in operations with tensors if it necessary for transition from one reference system to another. Application of multiplication of vectors for creation of dyads is inadmissible;
3. Tensor values define physical properties of elementary fluid particles, their geometrical deformations, kinematic properties and other dynamic processes in a continuous medium. Tensors take part both in addition operations with comparable tensors, and in multiplication operations with associated (dual) vector or scalar objects.

5.2 Construction of explicit numerical schemes

As input for construction of computer simulations in fluid mechanics the following dimensional fields in global reference system will be defined: $\{\vec{R}\}$ [m] – the field of mesh coordinates points; $\{\vec{V}\}$ [m/s] – the speed field; $\{\overset{<}{M}\}$ [kg] – the tensor field of internal properties for each of the fluid particles.

In thus defined mesh area local computing objects are introduced. Let us repeat physical parameters of fluid described elementary fluid particles: $\hat{r}$ [m^3] – tensor of large particle form; $\hat{v}$ [m^3/s] – tensor of local velocities of basis axes deformation of the particle; $\hat{f}$ [N m^2] – stress tensor at its boundaries.

In this case computer simulation could be divided into three stages (in language of tensor mathematics [12]):

Stage 1. KINEMATICS.

New field of nodal points:

$$\left\{ {}^{+}\vec{R} = \vec{R} + \vec{V} \cdot t + \vec{F} \cdot \overset{<}{M} \cdot t^2 / 2 \right\} \qquad (14)$$

The field of convective speeds is formed by algorithmic creation of the tensor:

$$\left\{ \hat{v} \right\} = \left\{ +\vec{V}\,i - o\vec{V}\,i \right\} \qquad (15)$$

Estimated status of the new field of internal properties:

$$\left\{ +\overset{>}{M} \right\} = \left\{ \hat{r} + \overset{\vee}{\rho} \right\} = \left\{ (\hat{r} + \hat{v}\cdot t)\cdot\overset{\vee}{\rho} \right\}$$

$$\left\{ +\overset{\vee}{\rho} \right\} = \left\{ \overset{\vee}{\rho}\cdot(\overset{\times}{1} + \overset{>}{v}\cdot t) \right\} \qquad (16)$$

Thus calculations of the distributed current characteristics are carried out on the fixed Euler mesh.

Stage 2. DYNAMICS.

The basis of this stage is satisfaction of physical conservation laws. Here comparison of fluid rheology with current state of computing model is carried out. E.g. let the momentum conservation law is defined $^{+}\overset{>}{M}\cdot\vec{V} = \overset{>}{M}\cdot(\vec{V} + {}^{\Delta}\vec{V})$. In this case basing (16) we have

$$^{\Delta}\vec{V} = (^{+}\overset{>}{M} - \overset{>}{M})\cdot\overset{<}{M}\cdot\vec{V} = \overset{>}{v}\cdot\vec{V}\cdot t \qquad (17)$$

and vector Newton equation (6) in Euler form that true for large fluid particle on fixed nodes of calculated area:

$$\vec{F} = \overset{>}{M}\cdot\overset{>}{v}\cdot\vec{V} = \hat{r}\cdot\overset{\vee}{\rho}\cdot\overset{>}{v}\cdot\vec{V}$$

The resulting expression contains fluid stressed state, which can be explained by the rheological properties of a computational model of the flow:

$$\left\{ \hat{f} \right\} = \left\{ +\vec{F}\,i - o\vec{F}\,i \right\} \quad \text{or} \quad \hat{f} = \hat{r}\cdot\overset{\vee}{\rho}\cdot\overset{>}{v}\cdot\hat{v} = \overset{>}{M}\cdot\overset{>}{v}\cdot\hat{v}$$

In a form of the new equation corresponds to record of stresses in the Navier-Stokes equations. Rheology of a real fluid is made in the form of laws (12), (13) associated with the tensor of convective velocities $\overset{>}{v}$.

Accounting of other conservation law restores loss of volume component of acceleration in the expression (17). It leads us to consideration of particle motion with variable mass without deformation.

$$\mathrm{M} = \det(\overset{>}{M}), \quad \rho = \det(\overset{\vee}{\rho}),$$

$$^{\Delta}\vec{V} = \vec{V}\cdot(\frac{M}{^{+}M} - 1) = \vec{V}\cdot(\frac{\rho}{^{+}\rho} - 1)\ . \qquad (18)$$

This model takes possibility to consider different stress modes. If we extract diagonal tensor $\overset{>}{v}_0$ in such a way that trace of residue $\overset{>}{v}^{*}$ is equal to zero:

$$\overset{>}{v} = \overset{>}{v}_0 + \overset{>}{v}^{*} \quad (tr\ \overset{>}{v}^{*} = 0)$$

than we obtain tensor of spherical compression:

$$\overset{\vee}{f}_0 = \overset{\vee}{\varepsilon}\cdot\overset{>}{v}_0\cdot t \qquad (19)$$

Selection of skew-symmetric part of a tensor gives viscous stress tensor:

$$\overset{\vee}{f}_H = \overset{\vee}{\mu}\cdot\overset{>}{v}_H = \overset{\vee}{\mu}\cdot(\overset{>}{v}^{*} - \overset{>}{v}^{*T})/2 \qquad (20)$$

The remaining symmetric tensor is associated with elastic deformation:

$$\overset{\vee}{f}_\Gamma = \overset{\vee}{c}\cdot\overset{>}{v}_\Gamma\cdot t = \overset{\vee}{c}\cdot(\overset{>}{v}^{*} + \overset{>}{v}^{*T})\cdot t/2 \qquad (21)$$

Full tensor of internal stress:

$$\overset{\vee}{f} = (\overset{\vee}{\varepsilon}\cdot\overset{>}{v}_0 + \overset{\vee}{c}\cdot\overset{>}{v}_\Gamma)\cdot t/2 + \overset{\vee}{\mu}\cdot\overset{>}{v}_H \qquad (22)$$

Dynamic coefficients $\overset{\vee}{\mu}, \overset{\vee}{c}, \overset{\vee}{\varepsilon}$ differ from kinematic coefficient by scalar density ρ., Particle has increment of internal movement velocity under the influence of the stress tensor:

$$^{\Delta}\overset{\vee}{v} = \overset{\vee}{f}\frac{t}{\rho} \qquad (23)$$

If flow is stable then tensor of speeds increment $^{\Delta}\overset{\vee}{v}$ has to compensate tensor of convective speeds for a calculated time interval:

$$\hat{v}\cdot\overset{\vee}{r} + \overset{\vee}{r}\cdot{}^{\Delta}\overset{\vee}{v} = 0$$

At this stage of the calculations, this expression is accurate, because it does not take into account the displacement of large particles in a time t.

Stage 3. STATIC.

At the final stage it is necessary to recover velocity field in accordance with increments calculated at the second stage. Here deformation movements around static centers of particles are considered. So during Lagrangian steps centers of gravity of large particles are shifted. We have to carry out interpolation of flow characteristics from these centers to initial nodes of computational area (Euler approach). At this stage it is possible to consider conditions on free boundaries. Here we use extrapolation with the help of centers of transborder fluid particles instead of interpolation in breaking nodes of nonregularized mesh.

For these purposes it is necessary to turn to mixed tensor from tensor $\overset{\vee}{v}$ defined in local basis. Mixed tensor is based on global reference system:

$$\overset{<}{v}=\overset{\vee}{v}\cdot\hat{r} \tag{24}$$

For transition to initial mesh the new local basis on the fixed knot is constructed. Spatial points shifted in time are used as adjacent nodes:

$$\hat{r}=\vec{R}_i-\vec{R}_i \tag{25}$$

Expanding expression (15) used in the construction of the tensor of local speeds on new basis vectors, we obtain algorithm for new velocity field calculation:

$$\vec{V}=\vec{V}+\sum_i \hat{r}\cdot\overset{\leftarrow}{v}_i \tag{26}$$

Expressions (23) - (26) reveal the basic algorithmic constructions allowing to apply inverse Newton's laws $\vec{W}=\vec{F}\cdot\overset{<}{M}$.

6. Conclusions

In the paper approach for constructing procedures for direct numerical experiment in problems of hydrodynamics is described. Distinctive feature of the proposed approach is a successful combination of well-known computing technologies (such as the "method of large particles" [3, 11]) and algorithms of tensor mathematics [8, 12]. We use dualism of corpuscular and continual representation of continuous medium (approaches of Euler and Lagrange). Introduction of a large particle with many degrees of freedom (movements, rotations, compression, stretching, etc.) makes it possible to consider the final transformation of computing object. This is very important, especially in problems of hydrodynamics, where even small effects can lead to significant displacement. The proposed approach makes it possible to exclude from consideration the mathematical models of fluid mechanics in the form of differential equations in partial derivatives. Construction on their basis of finite-difference computational schemes makes proceed from the consideration of infinitely small quantities (when considering the approximation of derivatives in the equations). In the proposed approach, computational experiment is carried out on the basis of fundamental conservation laws.

The dualism of corpuscular and continual models of continuous medium allowed to present computing procedure in the form of three serial stages combining approaches of Euler and Lagrange. Such division is aimed at providing efficient computing procedure especially in the conditions of the multiprocessor computer environment. As the basis of computational efficiency the use of explicit numerical schemes can be considered. This makes the internal state through control of the corpuscular-continuous computing environment possible. In this case application of hybrid or empirical solutions in subareas, where there is a violation of conditions of smoothness or stability of numerical schemes, is possible.

The apparatus of tensor mathematics is developed for construction of direct computing experiments on the basis of explicit numerical schemes. It fully describes physical processes in the continuous environment by means of the linear interpolation relations.

Experience in the application of this approach allows to judge the viability of historical ideas of Isaac Newton about corpuscular and continual construction

of laws of a mechanics of continua by means of finite differences – calculations of fluxions in three-dimensional space.

Acknowledgments

The research was carried out using computational resources of Resource Center Computer Center of Saint-Petersburg State University and supported by Russian Foundation for Basic Research (project N 13-07-00747) and St. Petersburg State University (projects N 9.38.674.2013, 0.37.155.2014). The authors thank Prof. Bogdanov for discussion of the problem and good ideas.

References

[1] Pletcher R.H., Tannehill J.C., Anderson D.A. Computational fluid mechanics and heat transfer. 3rd ed. CRC Press, Taylor&Francis Group, 2013

[2] Astarita G., Marrucci G. Principles of Non-Newtonian Fluid Mechanics. McGRAW-HILL, 1974

[3] Belocerkovski O.M., Davidov Yu.M. Method of large particles in gas dynamics. M.: Nauka, 1982 (in Russian)

[4] Lamb H. Hydrodynamics. 6th ed. Cambridge Univ.Pres., 1975

[5] Zommerfel'd A. Mechanics of deformable media. M.: Foreign Literature Publishing House, 1954 (in Russian)

[6] Kochin N.E. Vector calculus and beginnings of tensor calculus. 9th ed. M.: Nauka, 1965 (in Russian)

[7] Kilchevski N.A. Elements of tensor calculus and its application to mechanics. M.: Gostechizdat, 1954 (in Russian)

[8] McConnell A.J. Applications of Tensor Analysis. Dover Publications, 2011

[9] Faux I.D., Pratt M.J. Computational Geometry for Design and Manufacture (Mathematics and Its Applications). Ellis Horwood, 1981

[10] Methods in Computational Physics: Advances in Research and Applications, ed. by B.Alder, S.Fernbach, M.Rotenberg. Vol. 3: Fundamental Methods in Hydrodynamics. Academic Press, 1964.

[11] Hockney R.W., Eastwood J.W. Computer Simulation Using Particles. Taylor & Francis, 1989.

[12] Khramushin V.N. 3D Tensor Mathematics for the Computational Fluid Mechanics Experience. Vladivostok: FEB RAS, 2005 (in Russian)

[13] Monaghan J.J. Smoothed particle hydrodynamics. *Rep. Prog. Phys.* **68** (2005) 1703-1759

[14] Kitsionas S., Whitworth A.P. Smoothed particle hydrodynamics with particle splitting applied to self-gravitating flows *Mon. Not. R. Astron. Soc.* **330** (2002) 129–36

[15] Violeau D. Fluid Mechanics and the SPH Method: Theory and Applications. Oxford University Press, 2012

[16] Liu M.B. Smoothed Particle Hydrodynamics: A Meshfree Particle Method. World Scientific Pub Co Inc, 2003

[17] Degtyarev A.B., Khramushin V.N. Design and construction of computer experiment in hydrodynamics using explicit numerical schemes and tensor mathematics algorithms. *Mathematical Modelling* **26**, №11 (2014) (to be printed)

[18] Patankar S.V. Computation of conduction and Duct Flow Heat Transfer. Innovative Research Inc., 1991

[19] Ladyzhenskaya O.A. Mathematical Theory of Viscous Incompressible Flow. Mathematics and Its Applications Vol. 2. Gordon & Breach Science Publishers Ltd, 1969

[20] Ortega J.M. Introduction to Parallel & Vector Solution of Linear Systems. Plenum Press New York, NY, 1988

[21] The Fourth Paradigm. Data-Intensive Scientific Discovery. /ed. by T.Hey, S.Tansley, K.Tolle, Microsoft Research, Redmond, Washington, 2009

[22] Dubrovskii V.G., Bauman D.A., Kozachek V.V., Mareev V.V., Cirlin G.E. Kinetic models of self-organization effects in lattice systems. *Physica A*, **260** (1998), №3-4, p.349.

[23] Porubov A.V.; Maugin G.A., Mareev V.V. Localization of two-dimensional non-linear strain waves in a plate. *International Journal of Non-Linear Mechanics*, **39** (2004), i.8, 1359-1370

[24] Gankevich I., Gaiduchok V., Gushchanskiy D., Tipikin Yu., Korkhov V., Degtyarev A., Bogdanov A., Zolotarev V. Virtual private supercomputer: Design and evaluation. *Ninth International Conference on Computer Science and Information Technologies (CSIT). Revised Selected Papers, 2013*. IEEE Conference Publication, DOI: 10.1109/CSITechnol.2013.6710358

[25] Bogdanov A., Degtyarev A., Nechaev Yu. Parallel Algorithms for Virtual Testbed. *Proceedings of 5th International Conference «Computer Science & Information Technologies»*, Yerevan, Armenia, 2005, pp.393-398

Appendix

Let us introduce geometrical notations adopted in this work [12].

Local tensor in the absolute frame of reference is written as a string of three basis vectors or three-column coordinate matrix:

$$\hat{r} = \overset{\rightarrow}{r_i} = \begin{Bmatrix} \overset{\rightarrow}{r_1} & \overset{\rightarrow}{r_2} & \overset{\rightarrow}{r_3} \end{Bmatrix} = \begin{Bmatrix} r_{1,1} & r_{1,2} & r_{1,3} \\ r_{2,1} & r_{2,2} & r_{2,3} \\ r_{3,1} & r_{3,2} & r_{3,3} \end{Bmatrix}$$ (index at a vector on the right)

Projections of simple basis vectors of global coordinate system in local basis are represented uniquely in the form of dual basis $\overset{\vee}{r} = \overset{\leftarrow}{r^j} = \overset{\wedge}{r^{-1}}$ (or inverse matrix)

$$\overset{\vee}{r} = \overset{\leftarrow}{r^j} = \begin{Bmatrix} \overset{\leftarrow}{r^1} \\ \overset{\leftarrow}{r^2} \\ \overset{\leftarrow}{r^3} \end{Bmatrix} = \begin{Bmatrix} r^{1,1} & r^{2,1} & r^{3,1} \\ r^{1,2} & r^{2,2} & r^{3,2} \\ r^{1,3} & r^{2,3} & r^{3,3} \end{Bmatrix} = \overset{\wedge}{r^{-1}}$$ (index at a vector on the right)

$\vec{\boldsymbol{A}} = \vec{\boldsymbol{R}} + \vec{\boldsymbol{a}} = \boldsymbol{A}_i$ - the big vector with covariant components where the capital letter *A* means that a vector is constructed, measured relatively common center Ω and scaled in a uniform global coordinate system. If arrow is to the right → or subscript designate than vector components are projected on coordinate axes of global reference system. If arrow is to the left or vector index is at the top (superscript) $_{\Omega}\overset{\leftarrow}{\boldsymbol{A}} = {}_{\Omega}\boldsymbol{A}^{\boldsymbol{j}}$ then vector components are contravariant. They are projected in the dual system of local coordinates $\overset{\vee}{\boldsymbol{r}}$ inside large fluid particle. The one-to-one association between dual bases is defined by multiplication operation with tensor of form of concrete $\overset{\wedge}{\boldsymbol{r}}$ fundamental particle: $\vec{\boldsymbol{R}} = \overset{\wedge}{\boldsymbol{r}} \cdot {}_{\Omega}\overset{\leftarrow}{\boldsymbol{R}}$ or ${}_{\Omega}\overset{\leftarrow}{\boldsymbol{R}} = \vec{\boldsymbol{R}} / \overset{\wedge}{\boldsymbol{r}} = \vec{\boldsymbol{R}} \cdot \overset{\vee}{\boldsymbol{r}}$.

The left-hand indexes unless otherwise stated can be used for a space binding of computing object and for its mark in current time:

${}^{T}_{\Omega}\vec{\boldsymbol{R}}$ are *coordinates of knot point*. Ω defines location of node in mesh of computational domain; *T* is time from the beginning of the computational experiment.

${}^{t}_{+}\vec{\boldsymbol{R}}$ is *reference to adjacent point* (relative to the direction '+' starting from the center of mass of the large fluid particle Ω offset in time by an amount *t*).

$\vec{A} = A_i$ – space point (vector) marked in global coordinate system [m];

$\overset{\leftarrow}{a} = a^k$ – vector counting in the local basis of an elementary fluid particle [m-2];

$\hat{r} = \overset{\rightarrow}{r_k} = r_{ik}$ – tensor of form of large fluid particle [m3];

$\overset{\vee}{\rho} = \overset{\leftarrow}{\rho^j} = \rho^{kj}$ – tensor of density [kg·m-3];

$\overset{<}{M} = M^i{}_j = \overset{\vee}{\rho} \cdot \hat{r}$ – mixed tensor which relates the internal state of the particle at global reference system [kg];

In this case it is possible to present brief table of general notations

T – absolute time counting; $t = \Delta T$ – calculated time interval	c
p – pointwise (scalar) pressure	N/m^2
${}_{\Omega}^{T}\vec{R}$ – coordinates of knot of mesh area Ω at time moment T	m
${}_{+}^{+}\vec{R}$ – coordinates of adjacent point at the next time moment	m
$\vec{V}$ – full speed of fluid particle in global reference system	m/s
v – velocity vector relatively moving center of fluid particle	m/s
w – vector of velocity increment (*acceleration*) for fluid particles	m/s^2
$\hat{r} = \vec{r_k} = r_{ik}$ – geometric tensor of form large fluid particle	m^3
$v = {}_{\Delta}^{\Delta}r_i$ – tensor of local velocities (*velocities increment*)	m^3/s
$\overset{>}{v} = \hat{v}\,\overset{\vee}{r} = \hat{v}/\hat{r}$ – tensor of convective velocities	1/s
$\overset{\wedge}{\omega} = {}_{\Delta}\vec{V}_i$ – tensor of flows inside large fluid particle	m^3/s
$\overset{\vee}{\rho} = \overset{\leftarrow}{\rho^j} = \rho^{kj}$ – tensor of density or internal state of fluid particle	kg/m^3

$\overset{<}{\ }\ \overset{\vee}{\ }\ \overset{\wedge}{\ }$

$M = \rho \cdot r = M^i_j$ – tensor mass of fluid particle (mixed tensor resulting internal state of fluid to global frame of reference) kg

$\vec{F}$ – resultant vector of mass (volume) forces N

$\hat{f}$ – tensor of stresses at the boundaries of fluid particle N m^2

$\overset{>}{f} = \hat{f} \cdot r$ – stress inside and in a vicinity of fluid particle N/m

$\overset{>}{f}_H = \eta \cdot \nu_H / \Lambda$ – conditional tensor of viscous stresses

$\overset{>}{f}_\Gamma = c \cdot \nu_\Gamma \cdot t / \Lambda$ – conditional tensor of elastic stresses