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5 Современные задачи механики сплошных сред: новые математические модели, численные алгоритмы, результаты

5.1. *Belyayev Y., Kaltaev A., Naimanova A.* **2D Simulation of combustion in supersonic flow at the transverse injection of hydrogen**

Problem of interaction of hydrogen jet with supersonic air stream occur in the problems of modeling jet engine in rocket and space technology. It is very difficult to maintain (provide) combustion process in scramjet engine and it continues to be a very time consuming problem. Since the airflow is supersonic, fuel in the combustion chamber is remained a very short time (about 1 ms). During this short period of time, the fuel must mix with air at the molecular level and the chemical reaction and combustion should be completed prior to leaving the engine.

Simulation of nonpremixed turbulent combustion covers a description of the gas dynamic transport processes, diffusion process and mechanism of chemical reactions.

A mathematical model of this process is described by two-dimensional Reynolds averaged Navier-Stokes equations for multicomponent reactive gas. The turbulence model is defined by the algebraic model of Baldwin-Lomax. The mechanism of chemical reactions is described by seven reactions and seven components Spark's model.

The system of Reynolds averaged Navier-Stokes equations is solved using the ENO-scheme of the third order accuracy. Equations for the mass concentrations of chemical components are solved using the scheme of splitting by physical processes: the first step is calculated convective and diffusion transport using ENO-scheme, the second step of the matrix equation for the kinetic terms is solved implicitly.

5.2. *Chekmarev S.F., Kalgin I.V.* **Turbulent phenomena in protein folding dynamics**

Protein folding and hydrodynamic turbulence are two long-standing challenges, in molecular biophysics and fluid dynamics, respectively. The theories of these phenomena have been developed independently and used different formalisms. Here we show that the protein folding flows can be surprisingly similar to turbulent fluid flows. Studying a benchmark model protein (a SH3 domain), we have found that the flows for the slow folding trajectories of the protein have many properties of turbulent flows of a fluid. The flows have fractal nature and are filled with 3D eddies; the latter contain strange attractors, at which the tracer flow paths behave as saddle trajectories. Two regions of the space increment have been observed, in which the flux variations are self-similar with the scaling exponent $h = 1/3$, in surprising agreement with the Kolmogorov inertial range theory of turbulence. In one region, the cascade of protein rearrangements is directed from larger to smaller scales (protein net folding), and in the other, it is opposite directed (net unfolding). Based on the results of our study, we infer, and support this inference by simulations, that the origin of the similarity between the protein folding and turbulent motion of a fluid is in a cascade mechanism of structural transformations in the systems that underlies these phenomena.

5.3. *Chumakov G.A., Chumakov S.G.* **Canonical domains for almost orthogonal quasi-isometric grids**

A special class of canonical domains is discussed for the generation of quasi-isometric grids. The base computational strategy of our approach is that the physical domain is decomposed into five non-overlapping blocks, which are automatically generated by solving a variational problem. Four of these blocks – the ones that contain the corners – are conformally equivalent to geodesic quadrangles on surfaces of constant curvature, while the fifth block is a conformal image of a non-convex polygon composed of five planar rectangles (or a large rectangle with four small rectangles cut out of its corners). To ensure that the angles of the physical and canonical domains coincide and the conformal modules are the same, the four corner blocks are taken to be geodesic quadrangles on surfaces of constant curvature, namely, spherical, planar or Lobachevsky plane, depending on the angles of the physical domain. Within each of these blocks a quasi-isometric grid is generated. Orthogonality of coordinate lines holds in the fifth, central block.

We present an algorithm for automated construction of one-parameter family of such canonical domains. The parameter δ is defined in such a way that, according to a theorem that we have proved, for any physical domain there exists a unique value of δ for which the mapping from the canonical domain onto physical region is conformal and its derivative is bounded. Application of such a mapping results in a grid inside the physical region that is orthogonal far from the corners. This strategy ensures the existence of such canonical domain (the possibility to generate the grid) and the uniqueness of the mapping, i.e., our algorithm cannot converge to two different solutions. Note that the grid lines are the images of the geodesics in corresponding metrics.