ADVANCED STUDY CASES FOR NUMERICAL ANALYSIS*

FACULTY POSTER ABSTRACT

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A course on Numerical Methods typically covers introductory topics in numerical analysis for students of engineering, science, mathematics, and computer science who have completed elementary calculus, linear algebra and matrix theory. The course is usually limited to exploring basic algorithms for solving traditional simple problems in sciences and engineering [1]. As a result, the students have become inadequately prepared to construct and explore more sophisticated algorithms of modern technological challenges. To reduce this gap, the author has offered a series of study cases, which provide concrete examples of the ways numerical methods lead to solutions of some scientific problems. The similar approach was promoted in [2].

Various problems of applied mathematics, thermophysics, and aerodynamics (e.g., stability of mechanical systems and flow boundary layers, fuel combustion, and heat protection of space probes) come to solving differential equations with small coefficients at the highest derivatives. This phenomenon leads to the formation of regions with small linear dimensions where gradients of functions are large. The numerical analysis of such problems by traditional box-schemes is restricted by non-uniform convergence or even divergence of numerical solutions. In this study case, the numerical solutions of the model singular ordinary differential equation have been evaluated for the linear boundary value problem. The developed numerical method [3] was used for the analysis of gas flow parameters in boundary and viscous shock layers under the conditions of blowing on the body surface and nonequilibrium chemical reactions.

From a mathematical point of view, the increase of the flow rate of blowing gas or chemical-reaction rates is equivalent to the existence of a small coefficient at the highest derivative in the boundary-layer equations. A sublayer (of uncertain location) with large gradients of functions is created. The gas flow in the boundary layer was studied using a two-point exponential box-scheme and an effective regularization algorithm [3]. The uniform second-order convergence was obtained for functions and derivatives in the full range of small parameters such as blowing factors and inverse chemical-reaction rates. The approach could be applied to boundary layers with gas injection and combustion.

Many technological problems (e.g., calculations of transport coefficients and chemical-reaction rates) require estimations of multi-fold integrals under the conditions when classical Newton-Cotes formulas for numerical integration could not be applied. In the second case, students studied the rotational relaxation of a gas of homonuclear diatomic molecules. The realistic models of the intermolecular interaction [4] have been used for calculating the redistribution of the rotational and translational energies upon collision. To estimate the rotational relaxation time, the sixfold integrals were calculated at 200 points over the range of temperatures from 200 K to 10,000 K, using the Monte Carlo simulation technique, with 4000 tests at each point. The data for intermediate points were determined by means of the interpolation technique using cubic splines of defect 1 with smoothing. The accuracy of the calculations was estimated as 1.5%. The experimental data for molecular nitrogen correlates well with the numerical results.

The purpose of the third study case was to analyze heat transfer processes at the catalytic materials of the shock-tube end after shock wave refraction in terms of the model of the nonsteady-state nonequilibrium thermal boundary layer [5]. The major challenge was to develop the algorithm that could correctly and uniformly calculate flow parameters under all possible states (chemically "frozen", nonequilibrium, and equilibrium ones) right behind the moving reflected shock wave. The types of governing differential equations are significantly different in these three cases, and the algorithm should automatically "adapt" to these changes across the flow.

The system of algebraic-differential equations [5] was solved at each point of the flowfield behind the incident and reflected shock waves. A modified Newton's method with optimal choice of iteration step [5] was used for numerical solution of the equations. In the case of the initial pressure pl = 100 Pa, the flow behind the reflected wave is close to a state of local thermodynamic equilibrium, while in the other case pl = 1 Pa, the flow is significantly in nonequilibrium. The data were used as external boundary conditions for the flow parameters in the thermal viscous layer under the considered conditions.

The special topics covered mathematical foundations of evolution of dynamic systems that could be described in terms of attractors. The study cases of numerical modeling of the attractors of chaotic dynamical systems [6] (turbulence, weather forecast, and economic system development) also became a part of the course. They were introduced through classical examples of bifurcations of systems modeling equilibrium in chemical reactions (Rössler attractor) and atmospheric dynamics (Lorenz oscillator).

After brief in-class discussions of the study cases, each student continued working on a selected case as a project, created computer codes, run them at various parameters, compared the results with experimental data, and presented the findings to the classmates. In the course evaluations, students stated that they became deeply engaged in the course activities because they were examining the challenging problems.

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