New Possibilities of Computer Laboratory COMGA for Modelling of Convective Processes

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Requirements for a computer laboratory as for a system of physical processes modellingon PC are stated. Possibilities for computer laboratory for heat and mass transfer problems are described. It includes modelling of forced, natural and thermocapillary convection in ordinal and porous medium. A modulation of a body force is supplied aa well as a spatio-temporal body force behaviour, corresponding to space flight conditions. Applications include modelling of heat and mass transfer during crystal growth. System is approved on numerous test problems, including monotone and oscillating loss of stability, and could be considered as a certified new tool for training and study of general phenomena in heat and mass transfer, effectively extending handbooks possibilities.

1. Introduction

A solution of Navier-Stokes equations is one of a fundamental problem of modern mathematics and mathematical modelling of such systems is still some kind of art. While solutions of classical basic problems in fluid mechanics are governed by few non-dimensional parameters, a use of general packages of computational fluid dynamics for such problems study is connected with a need of large number data definition: region geometry, fluid properties, initial and boundary conditions, as well as a use of an arduous scheme: preprocessor-solver-postprocessor. Developed on intuitively clear for hydrodynamists principles, computer laboratory allows to make essentially easier and shorter a path from problem statement to results.

2. Computer laboratory: challenges and possibilities

Computer laboratory is based on a long-term experience of mathematical modelling of heat and mass transfer processes on a basis of Navier-Stokes equations in Boussinesq approximation [1, 2] and is treated as software modelling system COMGA for PCs [3-5].

A concept of computer laboratory includes possibilities to state and to solve general and classical problems of forced, natural and thermocapillary convection in both dimensional and non-dimensional terms, effective algorithms, allowing to make calculations in a real user time, in a combination with a visualisation, making an impression of a real laboratory experiment, an approbation on known solutions and international tests, a wide database of solved problems, a full access to a solution, friendly user interface.

COMGA includes possibilities of a solution of 2-D and axisymmetrical unsteady convective problems in rectangular enclosures, including modelling of Rayleigh-Bénard, Rayleigh-Taylor and Marangoni instabilities. A problem statement covers numerical models of essential number of papers for last few decades. A developing solutions database that confirms published experimental and numerical results in a combination with computer laboratory compose a basis for expert system in heat and mass transfer.

3. Problem statement

3.1. Governing equations

The unsteady Navier-Stokes equations in a Boussinesq approximation with equation of heat transfer and impurity are [1]:

$$\begin{aligned}
\mathrm{div}\vec{\boldsymbol{V}} &= 0 && (1)\\
\frac{\partial \vec{\boldsymbol{V}}}{\partial t} + (\vec{\boldsymbol{V}}\nabla)\vec{\boldsymbol{V}} &= -\nabla P + \nu\Delta\vec{\boldsymbol{V}} + (\beta_T T + \beta_C C)\vec{\boldsymbol{g}}(t) && (2)\\
\frac{\partial T}{\partial t} + \vec{\boldsymbol{V}}\nabla T &= a\Delta T && (3)\\
\frac{\partial C}{\partial t} + \vec{\boldsymbol{V}}\nabla C &= D\Delta C && (4)
\end{aligned}$$

where $\vec{\boldsymbol{V}}$, P, T, C, $\vec{\boldsymbol{g}}(t)$, t - correspondingly are velocity vector, dynamical pressure, temperature, impurity concentration, body force vector and time.

For modelling of space flight conditions a portable coordinate system, connected with space vehicle, is a non-inertial one and the motion equation (2) becomes

$$\frac{\partial \vec{\boldsymbol{V}}}{\partial t} + (\vec{\boldsymbol{V}}\nabla)\vec{\boldsymbol{V}} = -\nabla P + \nu\Delta\vec{\boldsymbol{V}} + \vec{\boldsymbol{r}} \times \frac{d\vec{\boldsymbol{\omega}}}{dt} + (\beta_T T + \beta_C C)\vec{\boldsymbol{n}}(t), \quad (5)$$

where $\vec{\boldsymbol{r}}$, $\vec{\boldsymbol{\omega}}$, $\vec{\boldsymbol{n}}(t)$ - are a point 3-D radius-vector relative to portable coordinate system, an absolute angular velocity of portable coordinate system, and full acceleration in a point, being calculated as

$$\vec{\boldsymbol{n}}(t) = \vec{\boldsymbol{r}} \times \frac{d\vec{\boldsymbol{\omega}}}{dt} + (\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{r}}) \times \vec{\boldsymbol{\omega}} + \frac{\mu_e}{|R|^3}\left[\frac{3(\vec{\boldsymbol{R}} \cdot \vec{\boldsymbol{r}})\vec{\boldsymbol{R}}}{|R|^2} - \vec{\boldsymbol{r}}\right] + \vec{\boldsymbol{a}}(t), \quad (6)$$

where μ_e, $\vec{\boldsymbol{R}}$, $\vec{\boldsymbol{a}}(t)$ are Earth's gravitational parameter, geocentric radius-vector of a center gravity of a space vehicle, aerodynamic force [6].

For a porous anisotropic medium the Boussinesq-Darcy equations are used.

3.2. Boundary conditions

Boundary conditions includes Dirichlet, Neumann and mixed boundary conditions for temperature and concentration. A region boundary is non-penetrative, a condition for tangential velocity corresponds either to an immovable or a driving lid or to a free surface with surface tension as linear function of temperature and concentration.

3.3. Body force modulation

The body force, being acted on fluid, is a combination of a permanent arbitrary directed part, harmonic vibrational and rotational parts and pulse part. The components of the body force could be read from a file.

4. Numerical model

For a solution of the equations a finite volumes method on staggered non-uniform meshes is used, it bases on explicit Chorin's projection method [7, 8] or semi-implicit SIMPLE scheme [9]. For solution of Poisson equation for pressure either an iterative method of successive over-relaxation (SOR) or a direct method based on combination of splitting and fast Fourier transform (FFT) in one of directions. An approximation of convective terms includes central differences, schemes with numerical viscosity of first order (upwind and hybrid) and of second order QUICK [8].

5. A use of computer laboratory

5.1. Problems classification

Problem statement in terms of computer laboratory is being realised either in terms of general model when one need to choose equations to solve, region geometry, fluid properties, boundary conditions, or by a choice of one of classified problems and a statement of few non-dimensional governing parameters. For classical Rayleigh-Bénard problem of heating from below there are three such non-dimensional parameters: aspect ratio, Prandtl number, Rayleigh number; other data will be defined by system. Definitely, the second approach is much more attractive and system efficiency is defined by a number of classified problems.

Problems classification includes:

- Forced convection

    Lid driven cavity

    Top- and bottom-lids driven cavity

- Natural convection

    Vertical layer with side heating

    Horizontal layer with side heating

    Rayleigh-Bénard problem

- Thermoconcentrational convection

    Layer structures (side heating)

    Layer with bottom heating

- Marangoni convection

    Pearson's problem

    Layer with side heating

    An interaction with natural convection

    Double Marangoni diffusion

- Convection under body force modulation

    Layer rotation (natural convection)

    Layer rotation (thermoconcentrational convection)

- Directional solidification

Moving front model

QSSM model

- Czochralski crystal growth

5.2. Example of use

A use of computer laboratory allows under simple examples to understand qualitive properties of liquid systems described by the Navier-Stokes equations, such as non-linearity, non-unique behaviour, loss of solution stability, hysteresis. As an illustration a study of a forced isothermal flow in a cavity with two oppositely moved top and bottom lids [10, 11] could be considered. There are two governing parameters in this problem: aspect ratio of cavity (H/L) and Reynolds number (Re) of moving lids.

Three different regimes of fluid flow are shown on fig. 1 for H/l=2, Re=100 (a), Re=3000 (b, c). At low Reynolds number Re=100 (fig. 1a) a fluid flow with two separate vertices of "sand-glass" type is realised. With increasing of Reynolds number up to 1700 two vertices are united into one main vertex, as on fig. 1b, with presence of two additional vertices of opposite direction. With consecutive decreasing of Reynolds number the one-vertex structure will remain down to Reynolds number equals 300, and then transforms into two-vertices structure again. So, within Reynolds number 300-1700 there is a hysteresis of solution: a type of solution depends on a path of parameter change. For Reynolds number equals 3000 one could obtain also another stable solution of a problem - non-symmetrical (fig. 1c). Its range existence is also limited by a value of Reynolds number from below - back transform to symmetrical state occurs.

5.3. Visualisation

Visualisation of physical processes occurs concurrently with modelling; process development could be seen on one of virtual screens, at each of them arbitrary number of windows could be created. Visualisation includes drawing of isolines, graphs of sections and time dependencies, fields of velocity vectors, animation of motion with test particles, creation of animated pictures, compatible with Internet-browsers.

5.4. Programming and system

Computer laboratory is developed in C++ in MS Visual Studio environment with a use of MFC library for user interface. That provides system functioning in MS Windows-9x/NT/2000/XP. For treatment of different applied models of fluid mechanics a mechanism of object-oriental C++ classes is used. Classes provide encapsulation (data hiding), inheritance, polymorphism (overdetermination and virtual functions). A structured database with modelling results and a public version of computer laboratory for tests reproduction is supplied in Internet [12] and could be used for a practical work treatment on numerical heat and mass transfer.

5.5. Union with laboratory experiment

Computer laboratory could be also effectively used in a combination with laboratory experiment, for example, for photoinduced soluto- and thermocapillary convection [13, 14], thermodiffusion [15] or physical convective practical work [16]. System could serve also as a tool for online analysis of gravitational sensitivity of heat and mass transfer processes on space station [6].

6. Tests description

During system development a special attention was paid for accuracy of numerical solutions. As except physical problem statement one needs an assignment of numerical parameters, a choice of which is very difficult to formalise, a test problems database is created where optimal numerical parameters is assigned. The tests allow to provide modelling within few minutes and could serve as a reference for close problems solution. Tests include a study of convergence of solutions on meshes and time steps, correspondence to international CFD tests [17-20], correspondence to data on monotone and oscillating stability loss of flows, obtained by solution on stability on eigenvalues.

6.1. Side heating in a square cavity

That is the first international test on numerical hydrodynamics [17] that corresponds to fixed temperature difference on vertical walls and adiabatic horizontal walls. In table 1 there is a comparison of a stream function maximum and Nusselt number on varied meshes with results in [17] (a difference in % are shown in brackets). On fig. 2 isolines of temperature and stream function for Rayleigh Ra=10^7 are present. For a linear distribution of temperature on horizontal walls a critical value of Rayleigh number, corresponding to oscillating loss of stability, equals to $1.7 \cdot 10^6$, that is close to an interval for critical Rayleigh number $1.8 \div 2.3 \cdot 10^6$ cited in [21].

6.2. Crystal growth

On fig. 3 a test result on directional solidification in presence of passive impurity, corresponding to calculation [22], Gr=5000, Pr=0.015, Sc=10, k=0.087, v_f=0.2 are present. On fig. 4 test results for an idealised Czochralsky crystal growth [19, 20, 23] for forced flows (a, b) and natural convection (c, d) cases are present.

Conclusions

Computer laboratory for modelling of heat and mass transfer is a principal new certified tool for study, training, results accumulation and presentation. Developing solutions database, bibliography and computer laboratory compose bases of expert system in heat and mass transfer.

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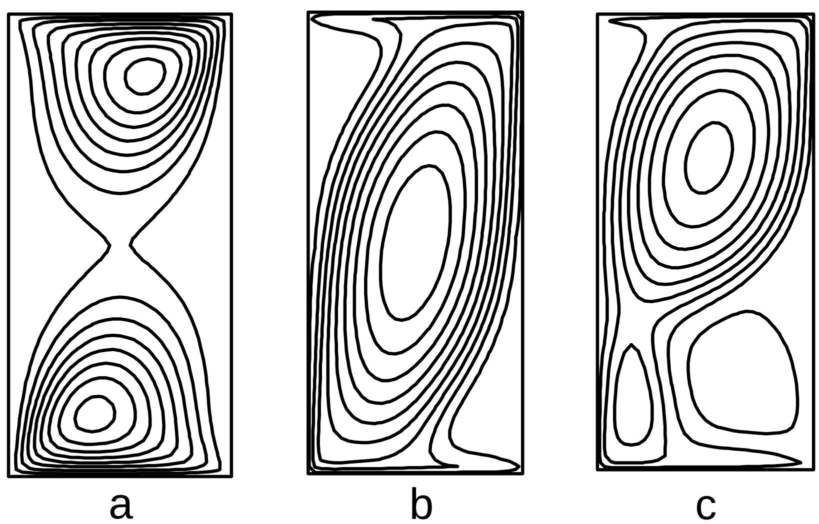

Fig. 1. A fluid flow structure (stream function) ina cavity H/L=2 with top and bottom moving lids for Reynolds number Re=100 (a) and symmetrical (b) and non-symmetrical (c) flows for Re=3000.

Table 1. A comparision of stream function maximum and Nusselt number for different meshes with results [17] for H/L=1, Prandtl number Pr=0.71,

Rayleigh number Ra=10^6.

Mesh	$\|\psi\|_{max}$	Nu
21x21	18.024 / **7.61**	10.518 / **19.29**
41x41	16.979 / **1.37**	9.052 / **2.67**
81x81	16.801 / **0.30**	8.854 / **0.42**
161x161	16.802 / **0.31**	8.829 / **0.14**
[17]	16.75	8.817

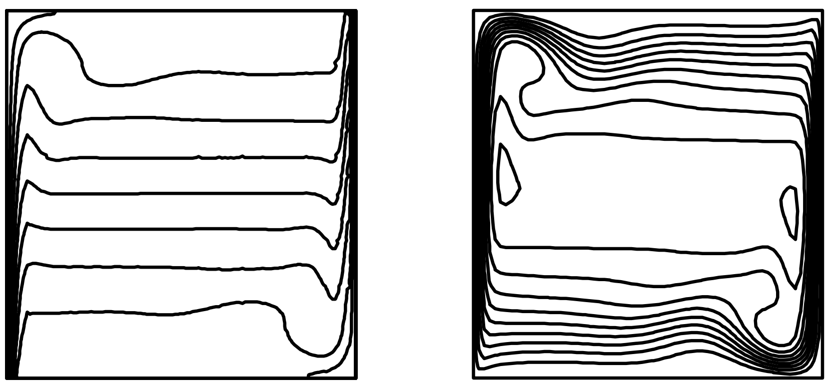

Fig. 2. Isolines of temperature (left) and stream function (right) for flow ina square cavity with side heating for H/L=1, Pr=0.71, Ra=10^7.

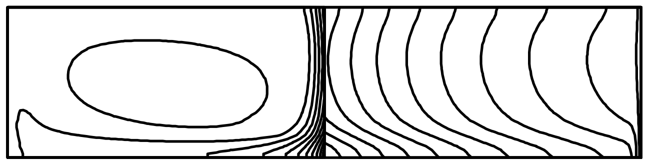

Fig. 3. Isolines of impurity concentration in a melt (left) and in a crystal (right).

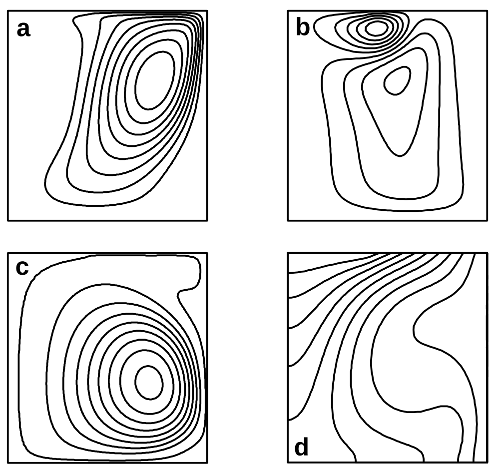

Fig. 4. Isolines of stream function for cases A3 (a), B2 (b), C2 (c) and temperaturefor case C2 (d) of [20].