On the concept of the interactive information and simulation system for gas dynamics and multiphysics problems

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Abstract. This paper describes the general idea and the first implementation of the Interactive information and simulation system – an integrated environment that combines computational modules for modeling the aerodynamics and aerothermodynamics of re-entry space vehicles with the large collection of different information materials on this topic. The internal organization and the composition of the system are described and illustrated. Examples of the computational and information output are presented. The system has the unified implementation for Windows and Linux operation systems and can be deployed on any modern high-performance personal computer.

1. Introduction
Progress in high tech strongly depends on the development of information and computing technologies. Such technologies are widely used in countries developing aircrafts (US, France, Japan etc.) for predicting their characteristics and for optimization of the parameters at the design stage, as well as for analysis of data at the stages of the ground and flight testing and for prognostic research on the subject. However, the accuracy of computations often doesn't meet modern requirements.

The latest achievements in supercomputer technologies and mathematical modeling of complex dynamic processes for atmospheric re-entry space vehicles make it possible to create computer models, the use of which will significantly reduce the amount of land and flight testing, lower the influence of the associated risks and improve the economic efficiency of finding optimal integral and engineering solution.

Currently there is no single software package for the complete multiphysical investigation of the interaction of a space vehicle with the surrounding gas. However, leading scientific institutions and design centers in the field of aerospace research have many years of experience and possess computer codes for solving different parts of this global problem [1-9].

Thus arises the problem of systematization and structuring of both existing and emerging computer codes into the single software package with a modular architecture that would allows to fully solve problems of modeling different sorts of interactions (mechanical, thermal, chemical) of a vehicle with the surrounding environment along the flight pass.

This integrated software package should include computational modules (solvers) for modeling the aerodynamics (aerothermodynamics) of prototypes of re-entry vehicles and their constructive elements, as well as the following tools and facilities:
for selection of a prototype model from the bank of prototypes;
for setting input data and computational parameters;
for selection, preparation and visualization of electronic surfaces and grids;
for querying physical and chemical characteristics of substances needed for the simulation;
for running a computation and controlling its progress;
for presentation and visualization of all kinds of the results (graphical, moving, textual, interactive);
for requesting and presentation of information resources on the topic of the simulation.

The goal is to eventually reach the world-class level of research in this area and surpass it in many ways. In particular, the new software package will allow to conduct the following research:

- to determine the aerodynamic and thermal loads on the surface and elements of perspective re-entry vehicles;
- to model thermogasdynamic processes in external and internal flows, taking into account the combustion;
- to model high-temperature flows in the shock layer near a vehicle with the integrated ramjet engine;
- to model interactions of high-temperature gases with the heat shield of a re-entry vehicle;
- to model unsteady flows in an integrated ramjet engine including the process of ignition in the combustion chamber;
- to simulate non-equilibrium chemical and photochemical processes and the formation of clusters and aerosol particles in exhaust jets of the engine;
- to model signatures of re-entry vehicles and ways of suppressing natural and artificial atmospheric disturbances.

The full-featured system of physical and mathematical models of the aerothermodynamics will allow to carry out numerical modeling of external configurations of re-entry vehicles as a whole and their key elements (edges of a body and wings, nose cone, engine) in particular. Simulations of key elements can be performed with higher accuracy to improve the reliability of the integral results.

This system will also provide access to a set of standard test problems formulated on the basis of ground and flight experimental data. These formulations can be used for performing preliminary calculations.

Additionally, a database on gas dynamics and multiphysics will be established in order to assist in performing numerical simulations and accelerate the study of external flows and physical processes in engines. This database will contain information about the physical-chemical properties of gases at high speeds, the kinetics of the combustion of fuel components, the thermal, thermodynamic and spectral optical properties of substances, as well as the catalytic properties of surfaces.

This paper presents the first variant of such integrated environment, the Interactive information and simulation system (IISS). Scientific and information content of the system is based on the experience acquired during the previous research in the fields of radiation gas dynamics, high speed aerothermodynamics and physical / chemical mechanics of non-equilibrium media and multi-temperature thermodynamics (see, for example, [4-9]).

2. Function and composition of the Interactive information and simulation system
Interactive information and simulation system considered in this paper is an integrated environment comprising computational modules with necessary input data, grids, information materials, scientific papers and reports on the themes of computational modules, collections of results of previous computations on these themes, databases on physical and chemical gas dynamics and other constituent parts. All these components are interconnected into a hierarchical / hypertext structure and form a unified information space. The system is organized as an integrated package with rich graphical user
interface. It can be deployed on a high-performance computer working under Windows or Linux operating system.

The IISS is driven by the interactive master control program which provides both the internal functionality of the system and the graphical interaction with a user. Graphical interface is implemented as a natural and convenient icon-based and menu-based environment. The master control program combines different tools and features which allow to provide the following capabilities:

- navigation through hierarchical and hypertext links;
- search and browse of information materials, papers and reports;
- view of graphical and video information, including surfaces and grids;
- query in databases and help subsystems;
- selection of a computational module and creation of a project to work with it;
- preparations for running a computational module (preview and editing of input data, selection and preview of a grid etc.);
- running a computational module, controlling the run, watching the output, stopping the computation;
- viewing textual and graphical results of the computation;
- launching external applications (table editors, graphical packages etc.);
- tuning and customization of the environment;
- user authentication and access control;
- accumulation of new results in the special database (not yet implemented);
- facilities for running computations remotely (not yet implemented).

3. Architecture of the interactive information and simulation system

Architecture of the IISS is based on the idea of separation of the code of the master control program from the application and information content. The graphical master program includes the above tools and features and is independent on the content of the IISS. It is controlled by the set of configuration files in XML format organized in the hierarchical manner. These files describe the structure of the application and information content of the IISS, appearance and layout of graphic elements on the screen, icons with their underlying functions, menus and other characteristics of the graphical interface. There is also another sort of configuration files which describe mechanisms and details of running application programs: nomenclature and types of input and output files, input data and options, grids, computational modules and scripts to run them.

Thus, the set of configuration files and scripts in conjunction with the directory tree containing all information and application data fully describes the whole content of the IISS and all working scenarios. Any modifications or additions of the content or scenarios are performed simply by editing or rebuilding configuration files and don't require to change and recompile the source code of the master control program. This ensures easy system expansion and development, e.g. addition of new prototypes and information materials, complication of operating scenarios, support of new external applications etc. Additionally, isolation of the master control environment from the data allows to implement several variants of the IISS with different application and information content in accordance with the specific needs of customers.

4. Description of the graphical interface and regimes

Graphical master control program of the IISS supports two main styles of the operation – the information regime and the computing regime. After the initialization and user's authentication, the system enters the information regime.
4.1. Information regime

In this regime, the screen is split into two fields – the upper one (menu field) with headings and icons corresponding to the objects to be selected, and the lower one (information field) with the descriptions of these objects and action buttons (figures 1 and 2). Clicking on an icon or action button either loads another screen (inferior with respect to the current one) with the similar organization, or performs some action (previewing a grid or a surface, browsing a paper or an information material, viewing a picture or a movie, opening a project for performing a computation etc.). There are also some navigation buttons (return, home etc.). All these control elements provide navigation in the hierarchical information space of the IISS. Owing to them, the user is able to browse information and illustrative materials to become familiar with the subject, to look through the previous computational or experimental results, and finally to create a new project for running a computational module.

Figure 1. Example of the information regime. Left-click on an icon (RAMC-2 or Fire-II) in the menu field loads the screen with the validation data, right-click switches to the computing regime.

Figure 2. Example of the information regime. Screen with the validation data for RAMC-2 experiment. Icons in the menu field represent information materials on the topic (papers and reports), action buttons in the information field switch to the screens with particular validation results.
The structure and content of the information space is mapped on the similar hierarchical structure of configuration files: each directory in the tree contains the XML file "dirinfo.dif" with the full description of each element or field on the screen (its layout, appearance, caption, associated action, name of an HTML file with the content of a field, link to the inferior directories, hypertext links to other elements etc.).

4.2. Computing regime

After clicking on a correspondent icon on the information screen, the system switches to the computing regime (figure 3). In this regime, a new field appears on the left side of the screen – project description tree (the remaining part of the screen retains the previous structure with the menu and information fields).

![Figure 3](image-url)

**Figure 3.** Example of the computing regime. Elements in the project description tree (left) represent the author’s abbreviation, working directory, input files and action button for starting a computation. Text in the information field (right) describes the working procedure.

A project description tree contains elements of two sorts – informative captions (passive) and actions (active). Elements may be organized into the hierarchical structure with the ability to hide subtrees (this is similar to the appearance of the file tree structure in typical file managers). Each active element is associated with some function, such as: initialize, create a working directory, set input options or parameters, view or edit an input file, read a description, select and view a grid, and finally start a computation (run a computational module).

After the computation is terminated (or stopped by the special button) new elements of the project tree may appear. These elements correspond to the results of the computation. Typically, they represent configuration files for graphical visualization (with predefined links to the files with raw results). By clicking on such an element, the corresponding graphical program (ParaView, Gnuplot, TecPlot etc.) is launched and outputs the results of the computation (see figure 4), with the ability of interactive manipulation with a picture (as appropriate). After watching these results, the user may repeat preparation actions (e.g. change input data) and run the computational module again.

Project trees are described by the special configuration files "*.prj" and "*.prs" (in XML format). These files contain all necessary information about each element, such as captions, associated actions and links.

The approach of the project description tree is very rich and flexible. It allows to organize complicated scenarios of the work without modifying the source code of the graphical master program. In particular, using the operating systems scripts (command files) allows to build dynamic
scenarios with accumulation of new results in the special database, as well as to support multiphase, multiuser, asynchronous (batch) and remote computations.

When the project description tree is open, it remains possible to work with the information field (on the rights side of the screen). After clicking on the correspondent navigation button, the system closes the project description tree and returns to the general information regime.

Figure 4. Examples of the computational results for RAMC-2 (left) and Fire-II (right) vehicles in the graphical form as obtained after clicking on the corresponding elements in the project description tree.

4.3. Other regimes

Besides two main regimes, the graphical control program supports several more subsystems:

- application-specific databases driven by the PostgreSQL database engine; they include data on the kinetics of the combustion, on kinetic parameters and transport coefficients, on spectral optical properties, on physical-chemical kinetics, on chemical reactions, on chemical kinetics of high-temperature gases and some others;
- interactive help subsystem; with the future extension of the information system, it will include descriptions of elements of the IISS and working regimes;
- grid manipulation and conversion utilities; currently this subsystem provides facilities for conversion of grids from different formats and for interactive 3D-view;
- administration and access control facilities; they are used to manage users and assign them different levels of privileges;
- system customization tools; they allow to define the location of the system, determine system utilities for dealing with different sorts of files (depending on the operating systems), rebuild configuration files etc.

The diagram on figure 5 illustrates the structure and content of the IISS (in the simplified form). In this example, the user selects FIRE 2 space vehicle as a particular case of the prototype P1, specifies the small grid for this vehicle, previews it and then creates the project description tree in order to run Code 1. Elements of this tree illustrate phases of the further computational session.

5. Implementation of the graphical master control program

The master control program of the IISS is written on C++ language. The graphical interface is implemented using the open-source cross-platform application framework Qt [10, 11], version 5.5.
Figure 5. Example of the structure and content of the Interactive information and simulation system.
The program can work on the Microsoft Windows as well as on different variants of Linux. System-dependents parts of the code use "ifdef" and "ifndef" constructs to distinguish between Windows and Linux, thus the source code is unified. Total length of the current variant of the program exceed 5000 lines of code.

Computational modules can be written on any programming languages and compiled by any suitable compilers. Modules are launched indirectly from within command files (scripts). There are two sets of scripts – for Windows (files "*.bat") and for Linux (Bash scripts). If some module needs a run-time library, the required environment can be established inside the corresponding script. Similarly, a complex running procedure can be algorithmized within a script also (e.g. running a parallel job with the use of OpenMP and/or MPI environment). Generally, the script approach allows to release the master control program from doing complicated actions and particular tunings.

6. Conclusion
The presented interactive information and simulation system and its main element, graphical master control program, provide integration of computational modules, grid manipulation tools, information resources and other elements into the unified information and computational environment. The system is being extended continuously, both by adding application modules (solvers) accompanied with corresponding information elements (papers, documents, visual elements, results of computations), and by enhancing the capabilities of the master control program. The resulting computational platform will become the efficient and convenient technological and educational environment for performing computations, visualization and analysis of results for gas dynamics and multiphysics problems.

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