Keldysh Institute of Applied Mathematics
of Russian Academy of Sciences

Web Laboratory for Supercomputer Simulation of Deposition Processes

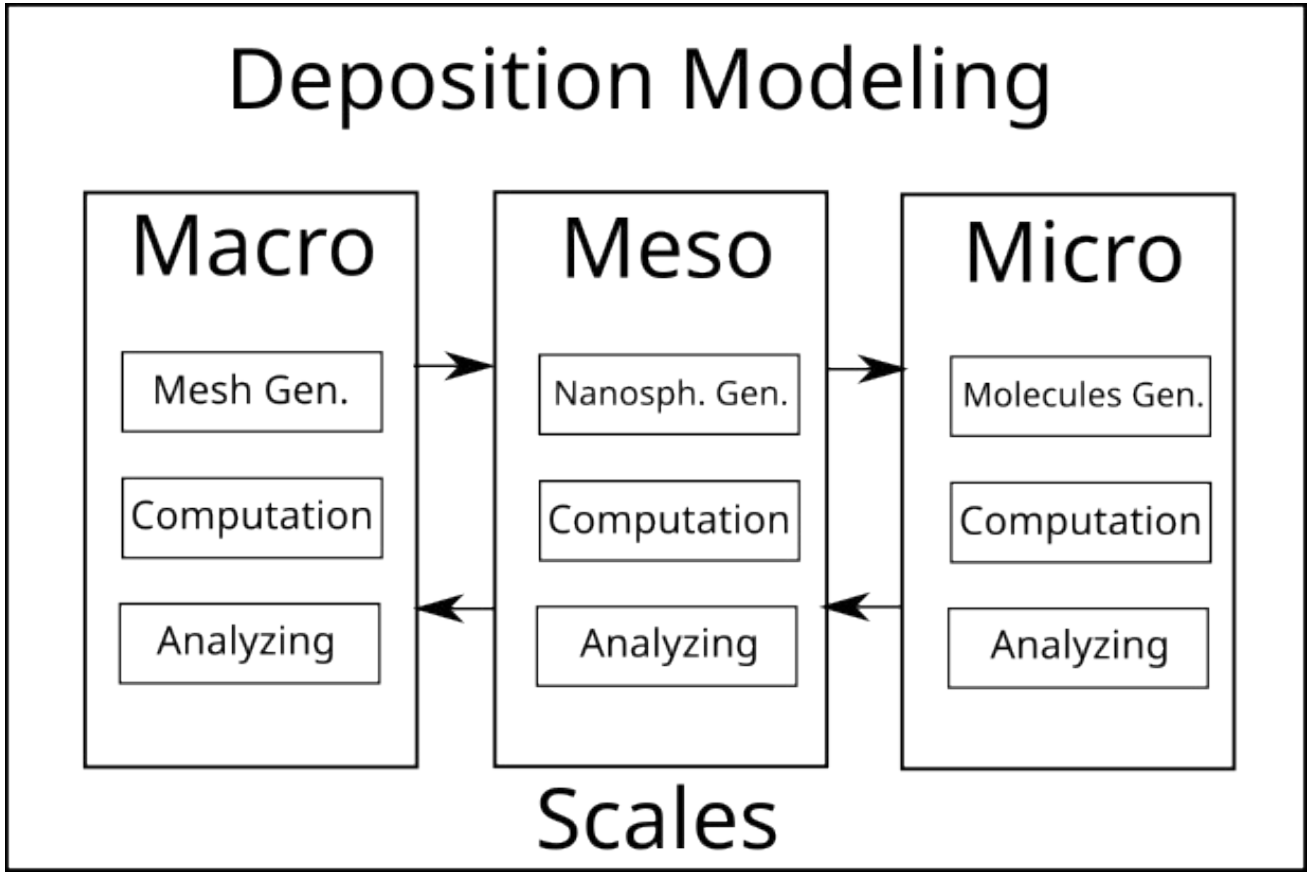
Tarasov N.I.*, Podryga V.O., Polyakov S.V.

*e-mail: nikita_tarasov@imamod.ru

10th International Conference «Distributed Computing and Grid Technologies in Science and Education» (GRID'2023), 3-7 July 2023, Dubna, Russia

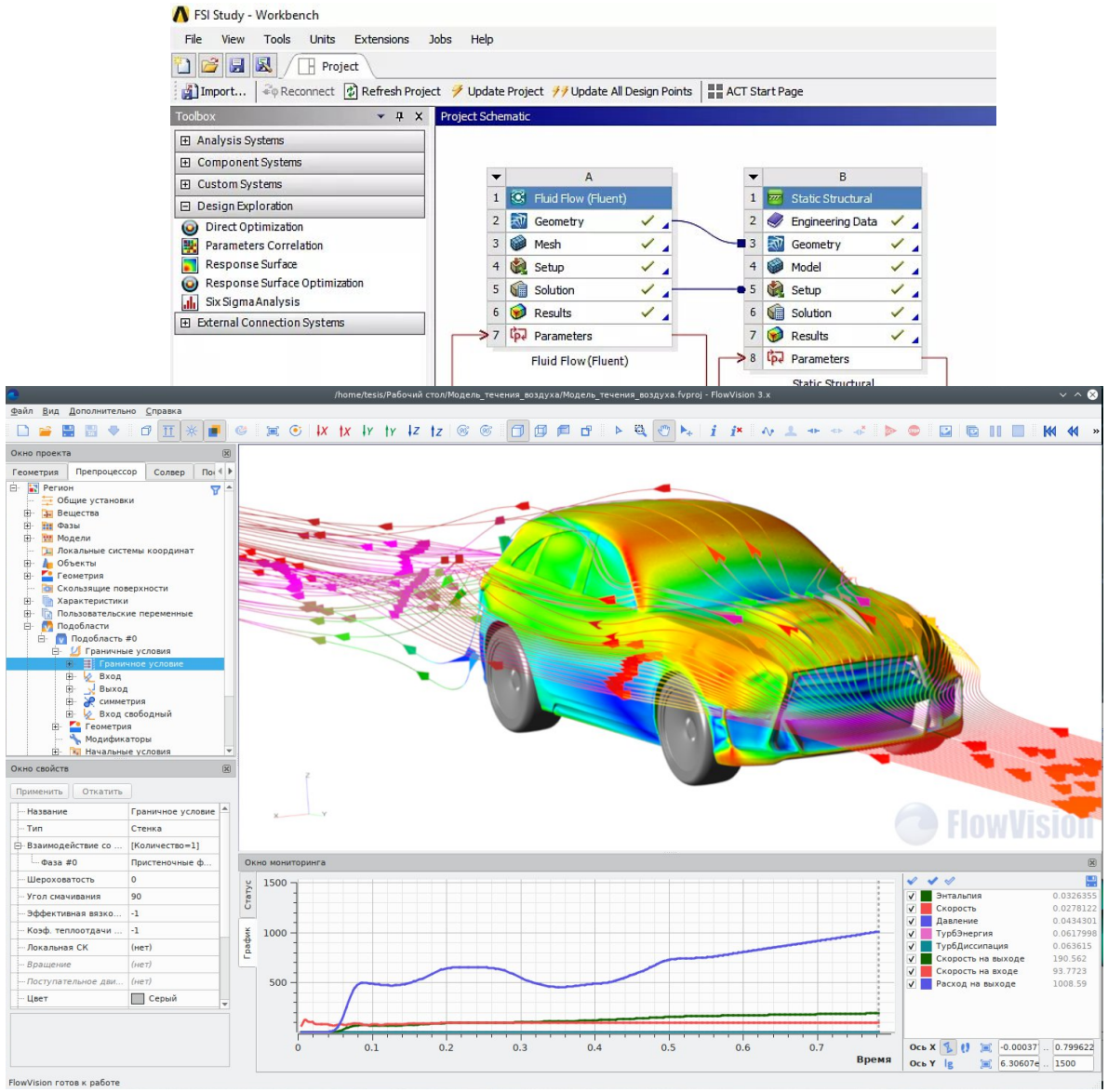
Relevance

- Mathematical models elaboration leads to an increase in the number of applied approaches and methods
- The number of applications and it’s computational complexity are increasing
- Complicated inter-program exchanges and tasks management on the computer
- The storage, cataloging and analysis of the results of experiments becomes more complicated



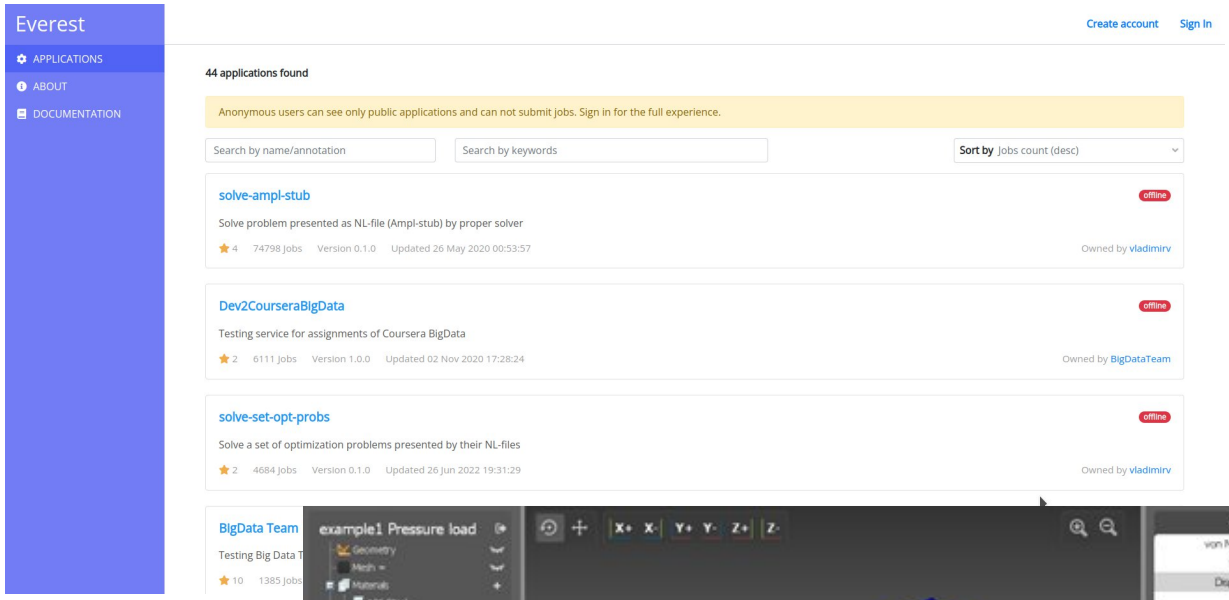
Main goals

- Unification of a interaction with remote computing resources
- Unification of a applications preparation for computational experiments
- Providing the ability to manage and track the progress of user tasks in graphical interface
- Unification of storage, access and analysis of the computational experiments results



Web laboratories

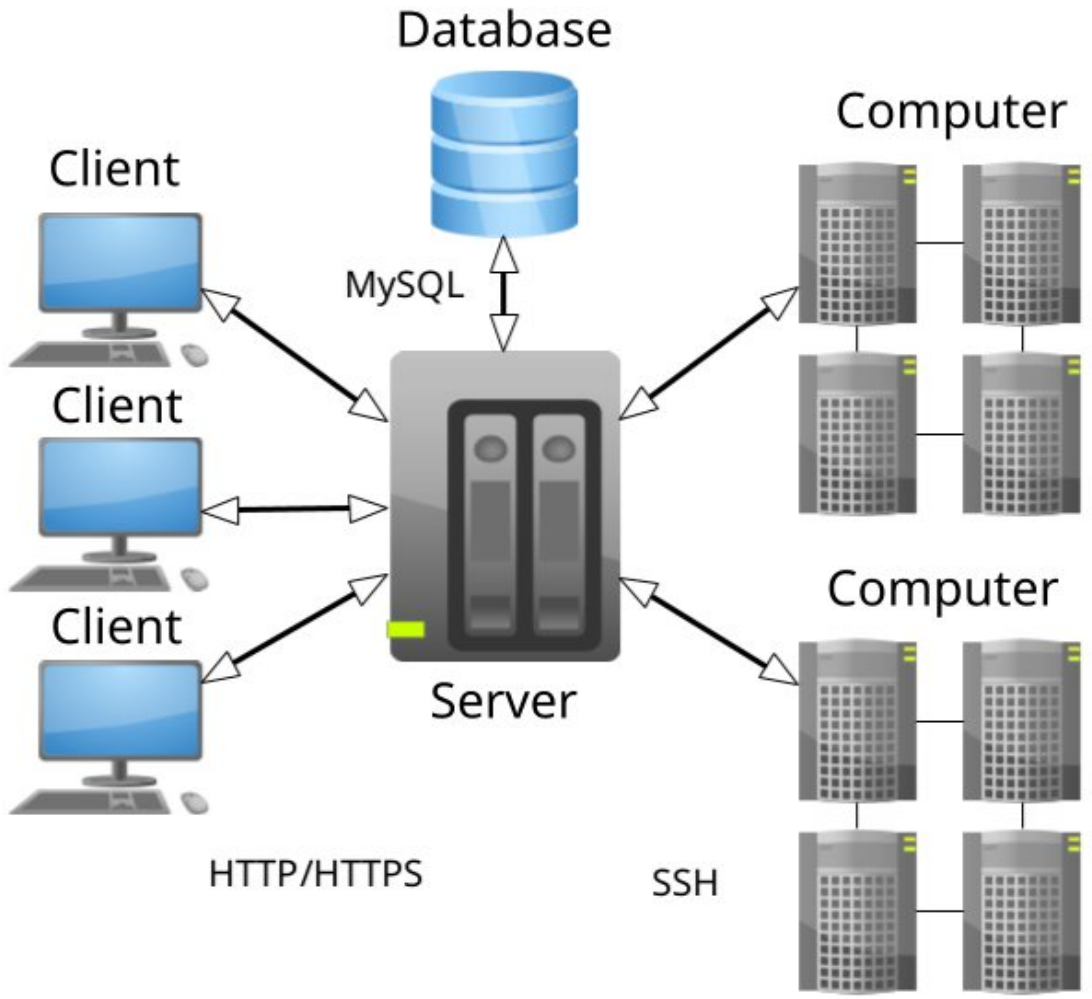
- Domain specific web laboratories have a rich and responsive GUI[1,2]
- Generalized web laboratories have ability to integrate third-party applications[3]



[1]https://www.sim4design.com
[2]https://nucleonica.com/
[3]Sukhoroslov O., Volkov S., Afanasiev A. A Web-Based Platform for Publication and Distributed Execution of Computing Applications // 14th International Symposium on Parallel and Distributed Computing (ISPDC). IEEE, 2015, pp. 175-184

Digital platform

- Client-server application
- User access to the server through a web browser via HTTP/HTTPS protocol (with websocket usage)
- MySQL database for storing meta data
- SSH access to supercomputers with the ability to dynamically add new entries



Technology stack

Programming language:

- TypeScript

Server:

- Node.js
- Express.js
- TypeORM

Client:

- Vue.js
- Quasar

TYPEORM

Express

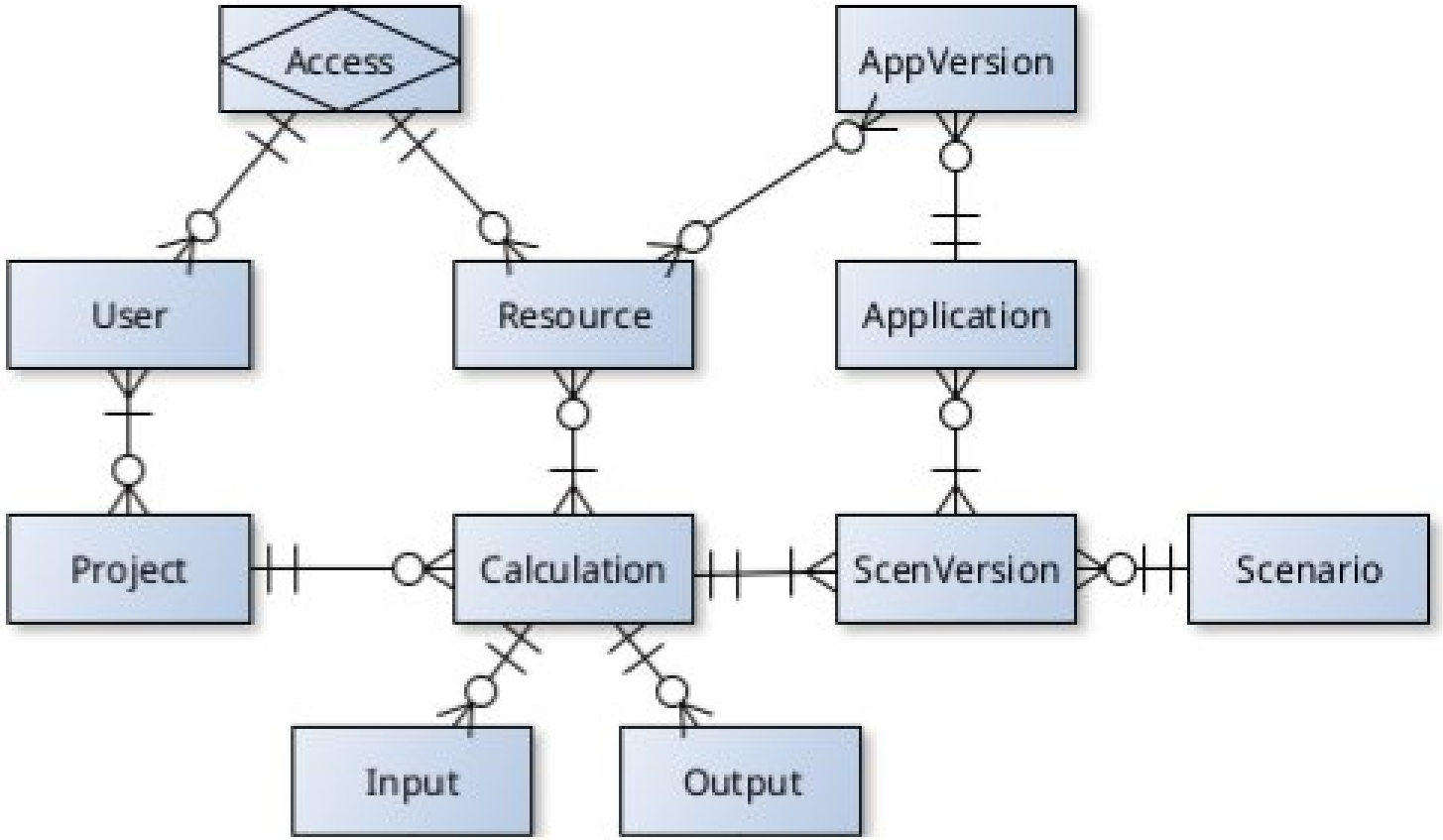
Vue.js

QUASAR

BEYOND THE FRAMEWORK

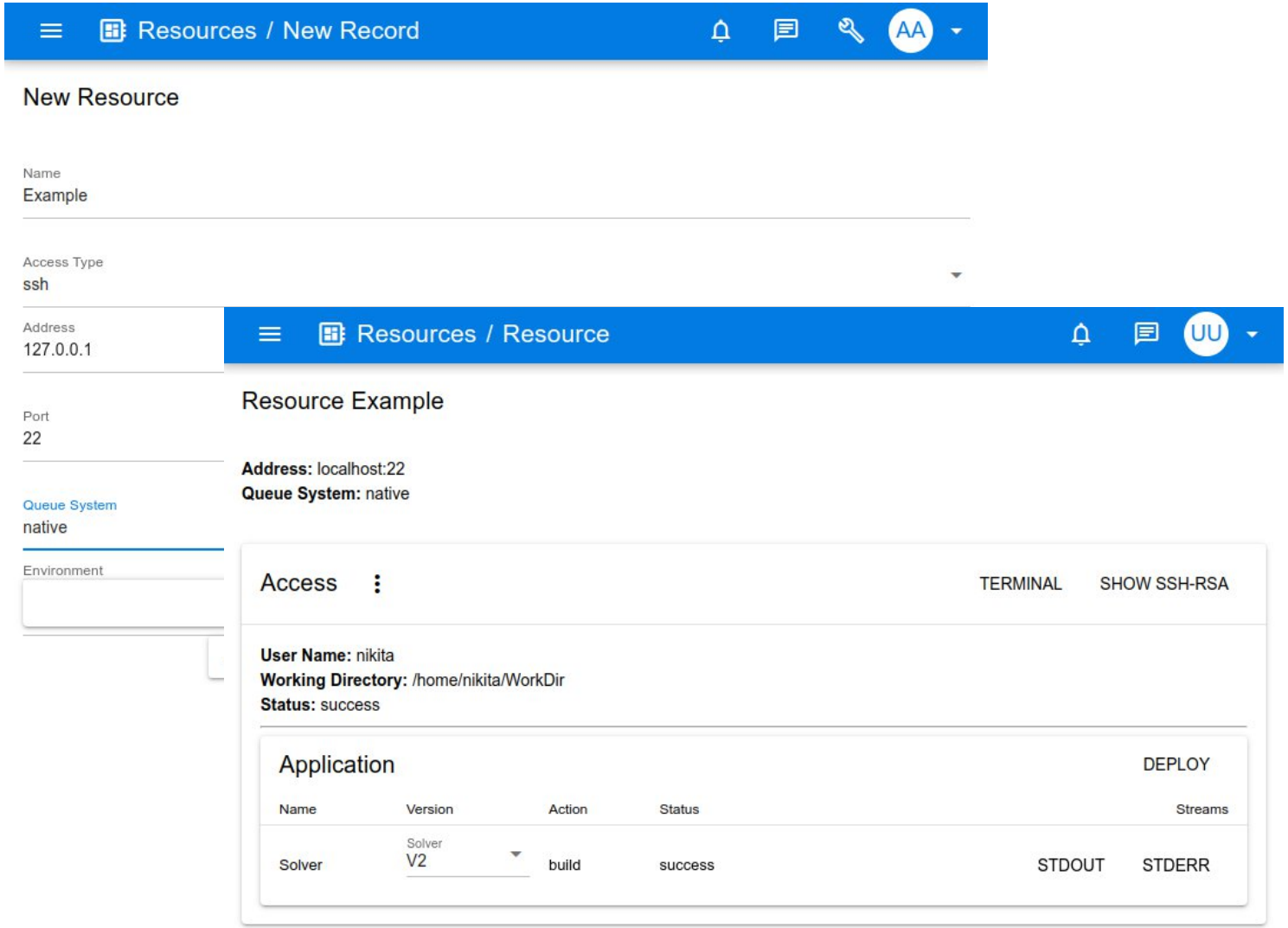
Database

- User
- Resource
- Access
- Application
- Scenario
- Project
- Calculation



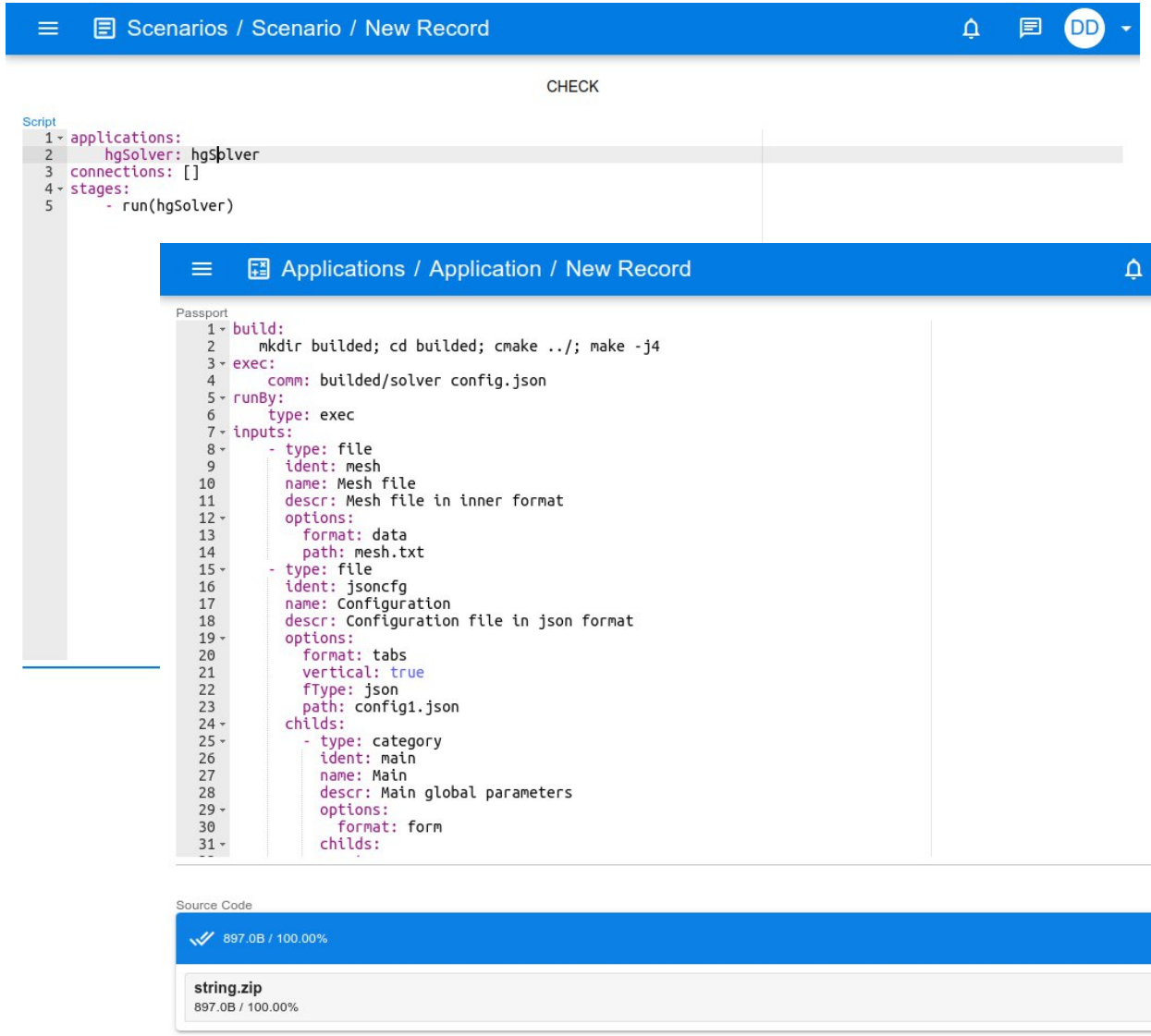
Computing resources

- Resource is a representation of a remote supercomputer. Includes: IP or hostname, port, task queue system type
- Access is a representation of the user-resource relationship. Includes: username, home directory, personal rsa-keys



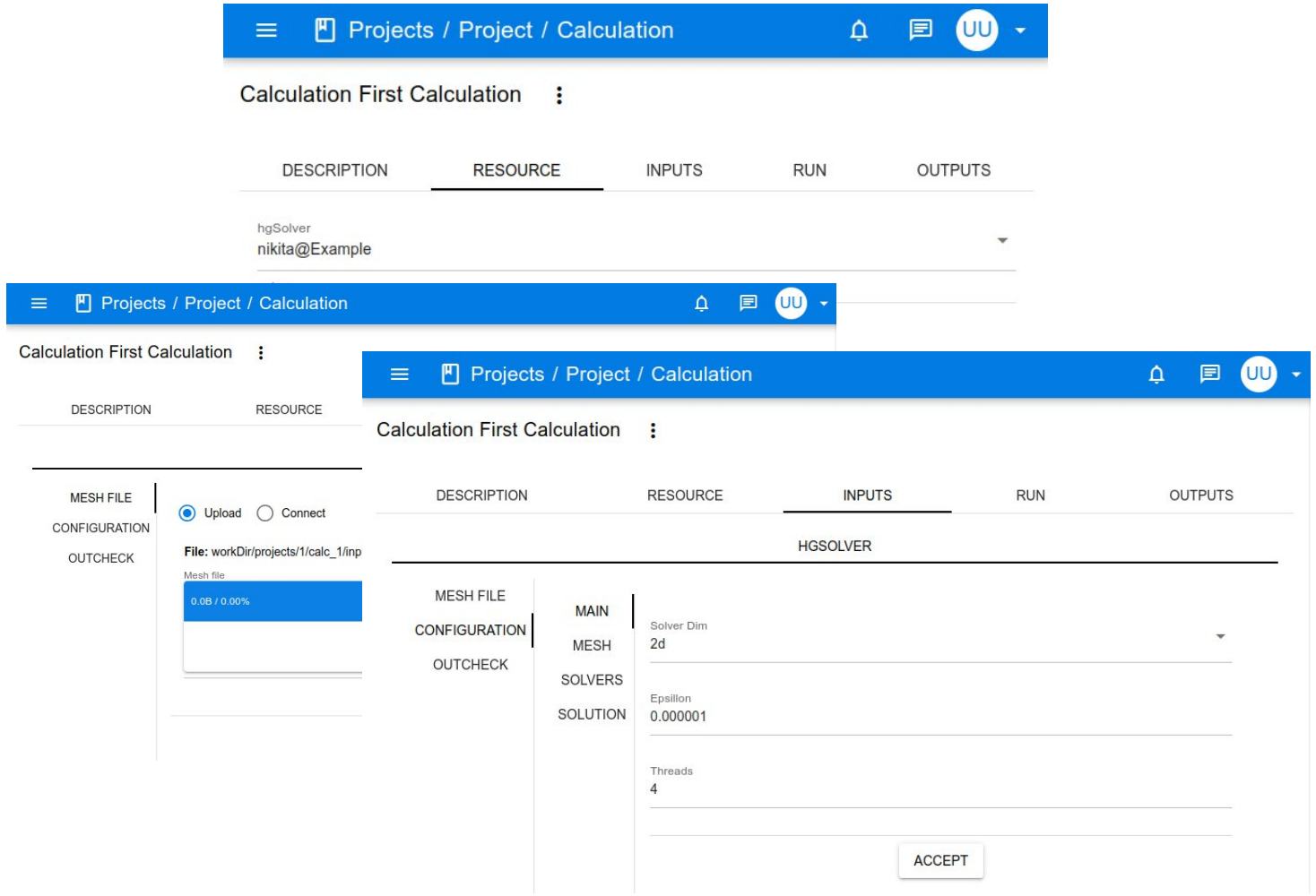
Applications integration

- Application is representation of the programs in the web laboratory. The main meta-information is in the application passport in yaml format, includes: build and run commands, description of the input parameters and output data
- Scenario is a representation of the applications set aimed at solving a specific problem. Meta-information in yaml format includes: description and order of launching applications, internal links of output and input data



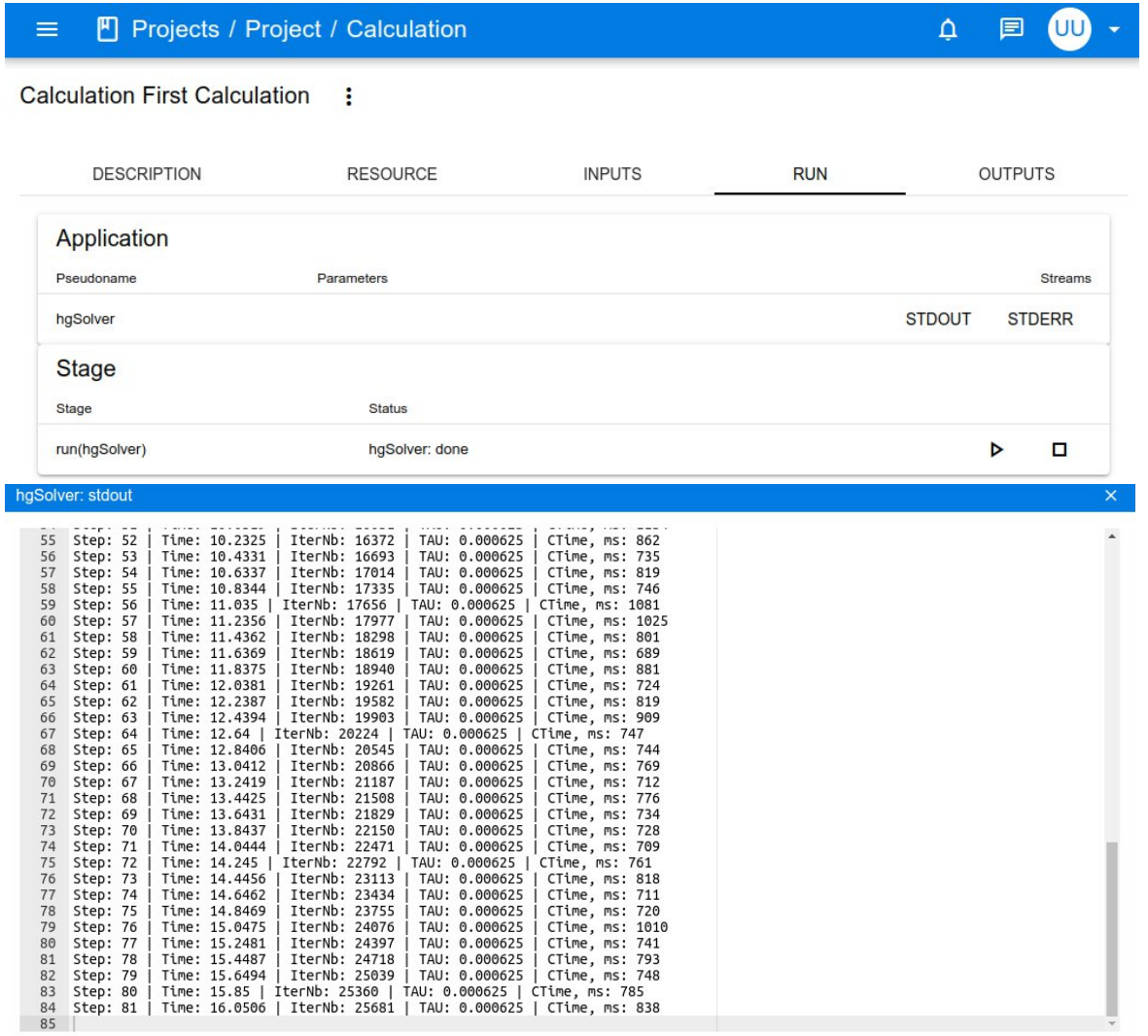
Computer experiments. Preparation

- Project is a combination of computational experiments. Includes: text description and set of calculations
- Calculation is a functional part of the platform and represents computational experiment. It provides: preparation, configuration and run of the applications, storage and access to the results



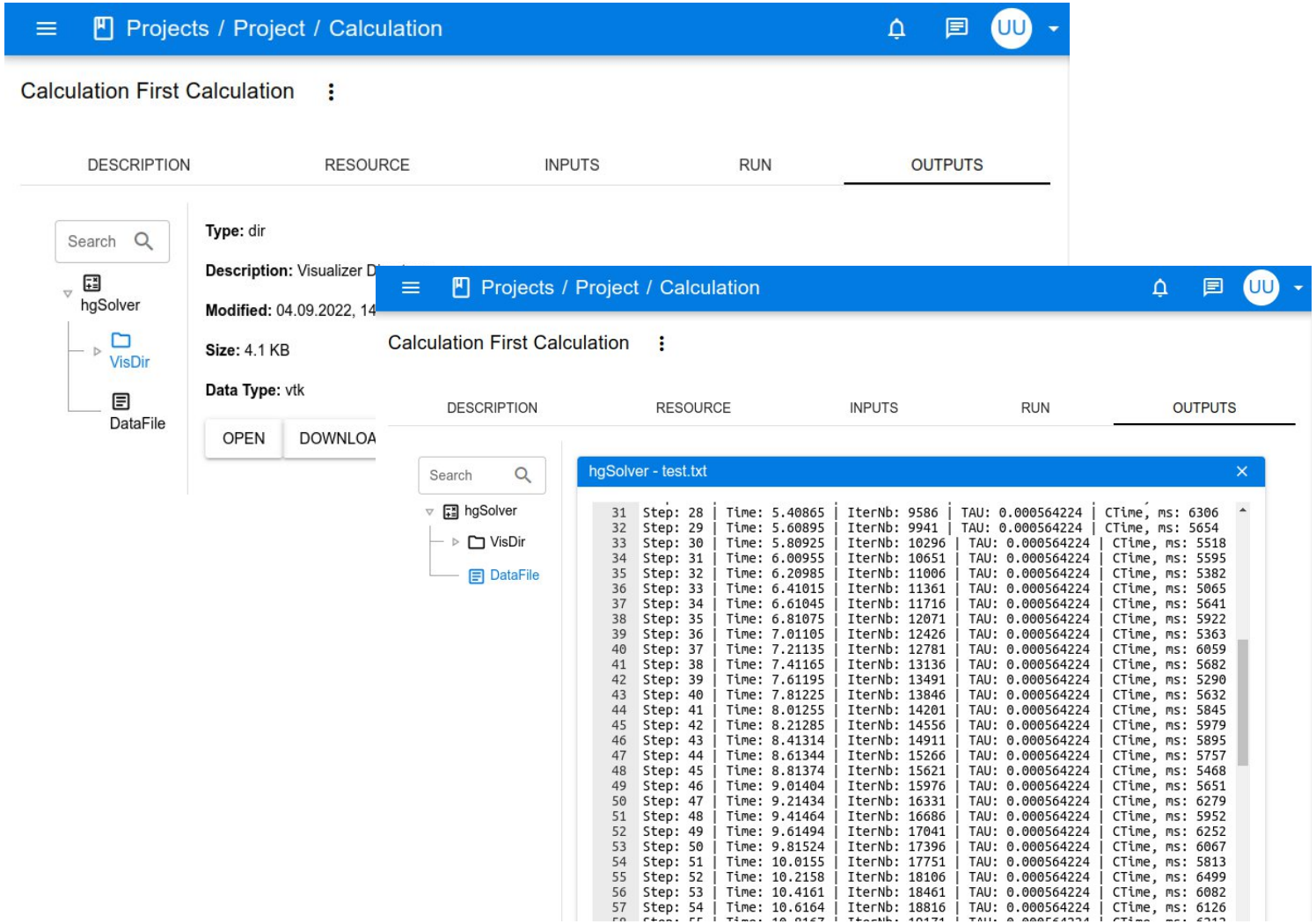
Computer experiments. Tasks

- Task is a representation of user tasks on a remote computer. Includes: unique task ID, current status in the queue
- Digital platform allows starting and stopping jobs, access to standard I/O streams



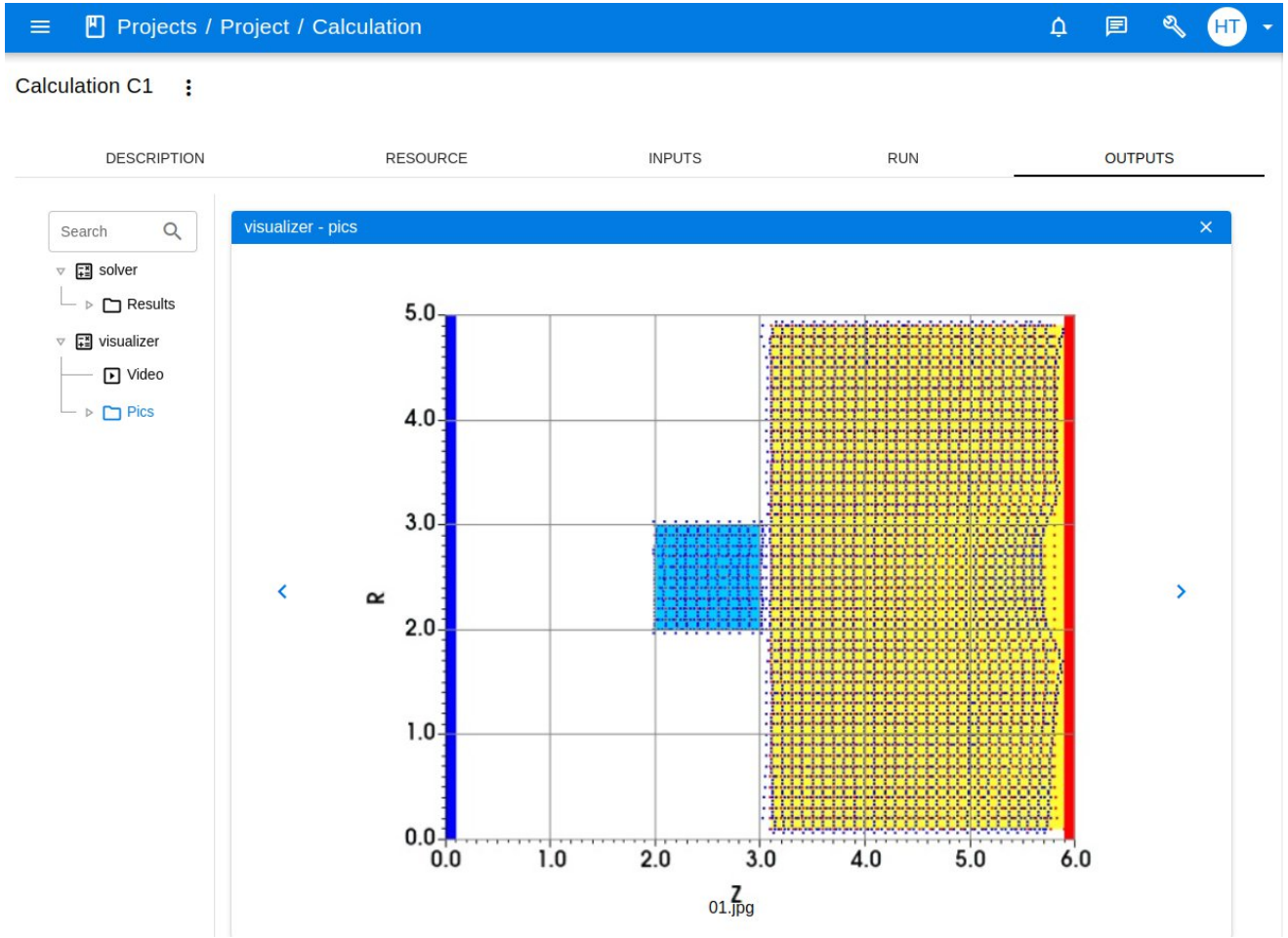
Numerical results analyzing

- Analysis of the results of a computational experiment is carried out using the following approaches:
  - direct access to text data files, pictures and videos
  - non-interactive analysis and rendering of data into image files
  - interactive “in-web” visualization of data files



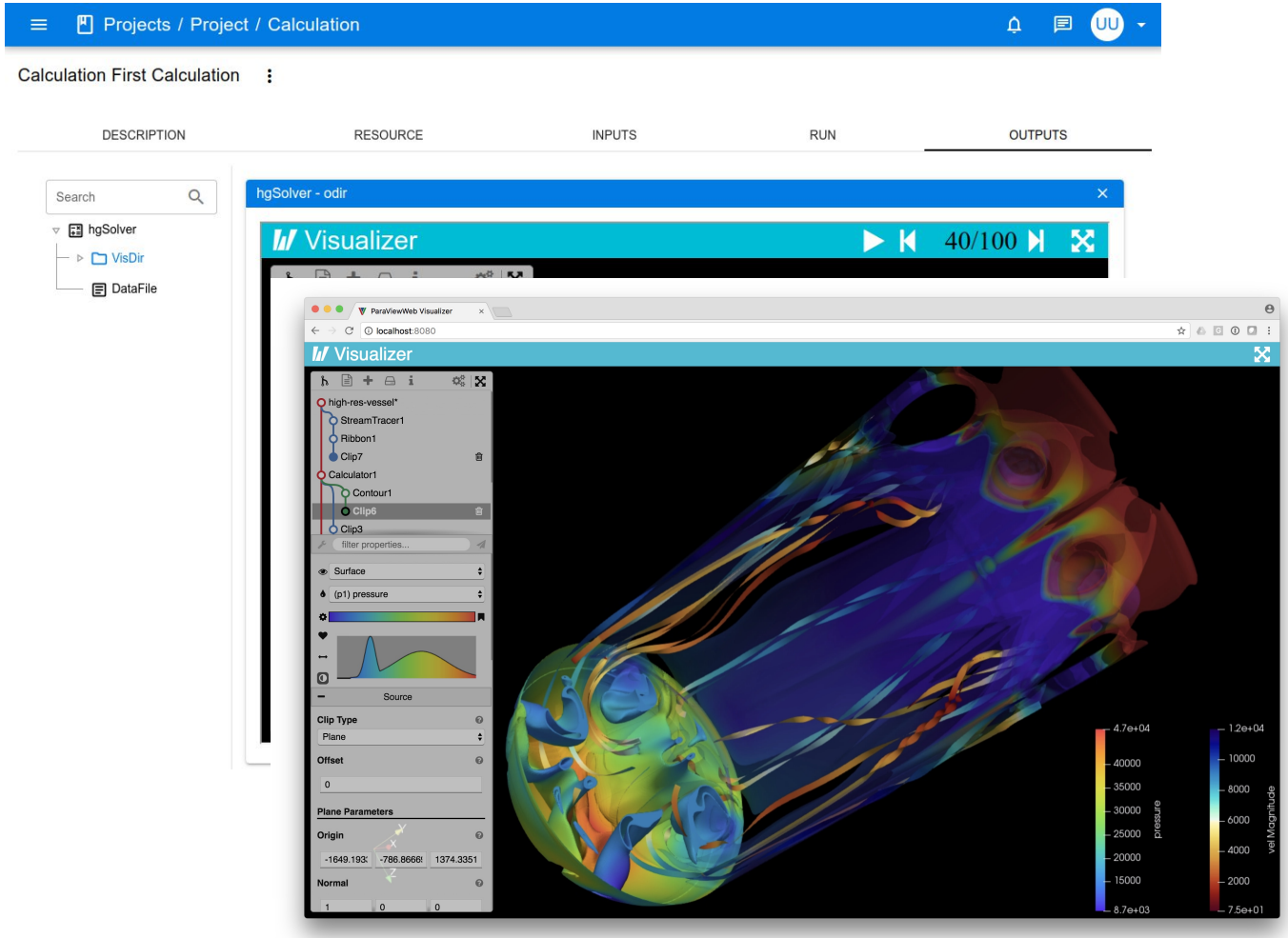
Resource-side analyzing

- Interaction with output data allows direct display of images and movies generated from data files via processing utilities on a remote computer
- The digital platform allows the developer to embed the necessary data processing utilities



Interactive visualization

- Direct interactive visualization of data files. It is possible to use the following approaches:
  - Embedding of Kitware Visualizer[1]
  - Developing original GUI to ParaViewWeb server[2]



[1]https://kitware.github.io/visualizer/
[2]https://kitware.github.io/paraviewweb/index.html

Conclusion

- The peculiarities of applying complex mathematical models are considered
- The web laboratories approach to simplify the application of complex models is proposed
- The architecture of the digital platform and the stack of technologies for its implementation are proposed
- Preliminary implementation of the web laboratory for supercomputer simulation of deposition processes has been implemented

The work was carried out with the support of the Russian Science Foundation, project No. 21-71-20054

Thank you for your attention!