

Keldysh Institute of Applied Mathematics
of Russian Academy of Sciences

Web Laboratory for Supercomputer Simulation of Deposition Processes

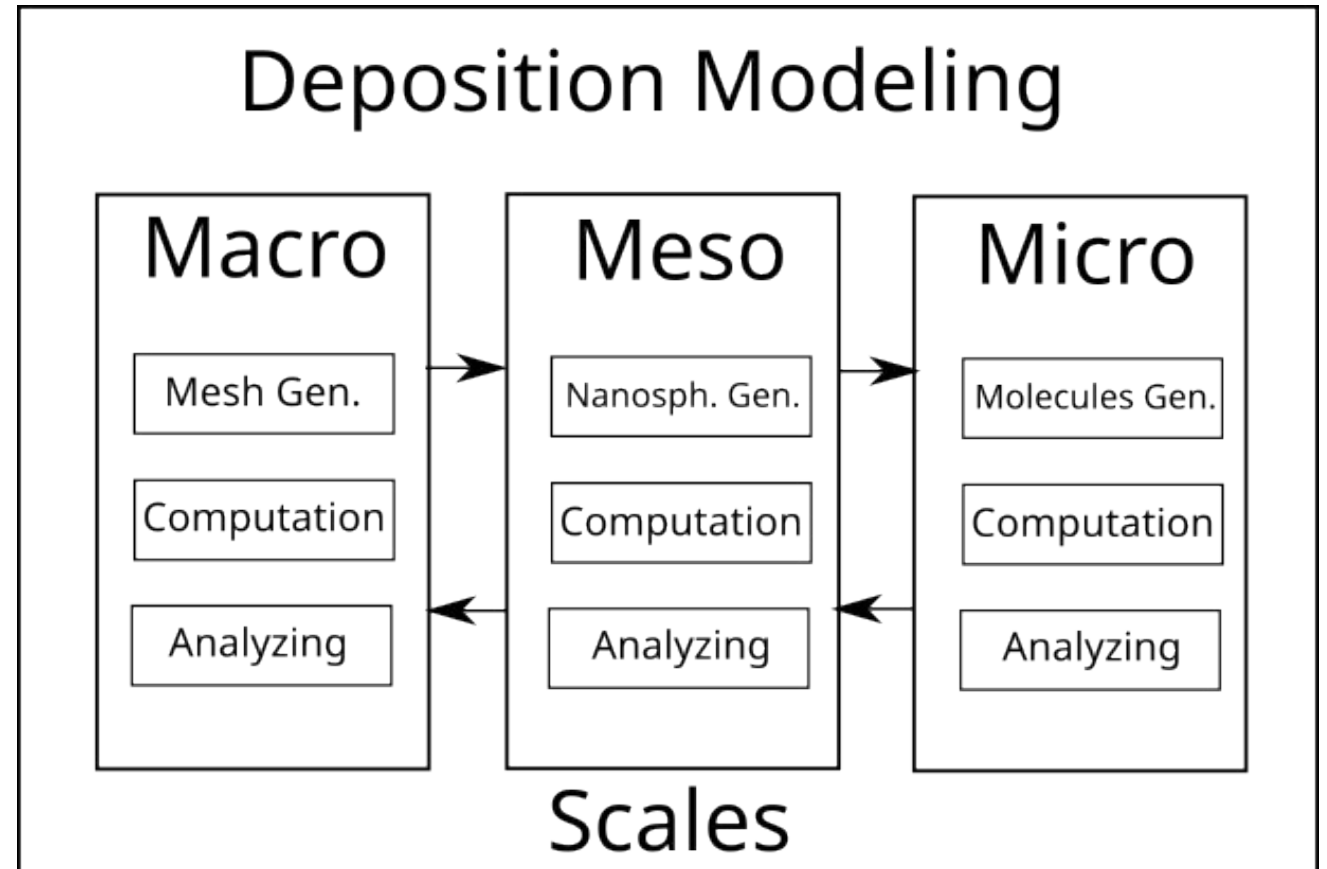
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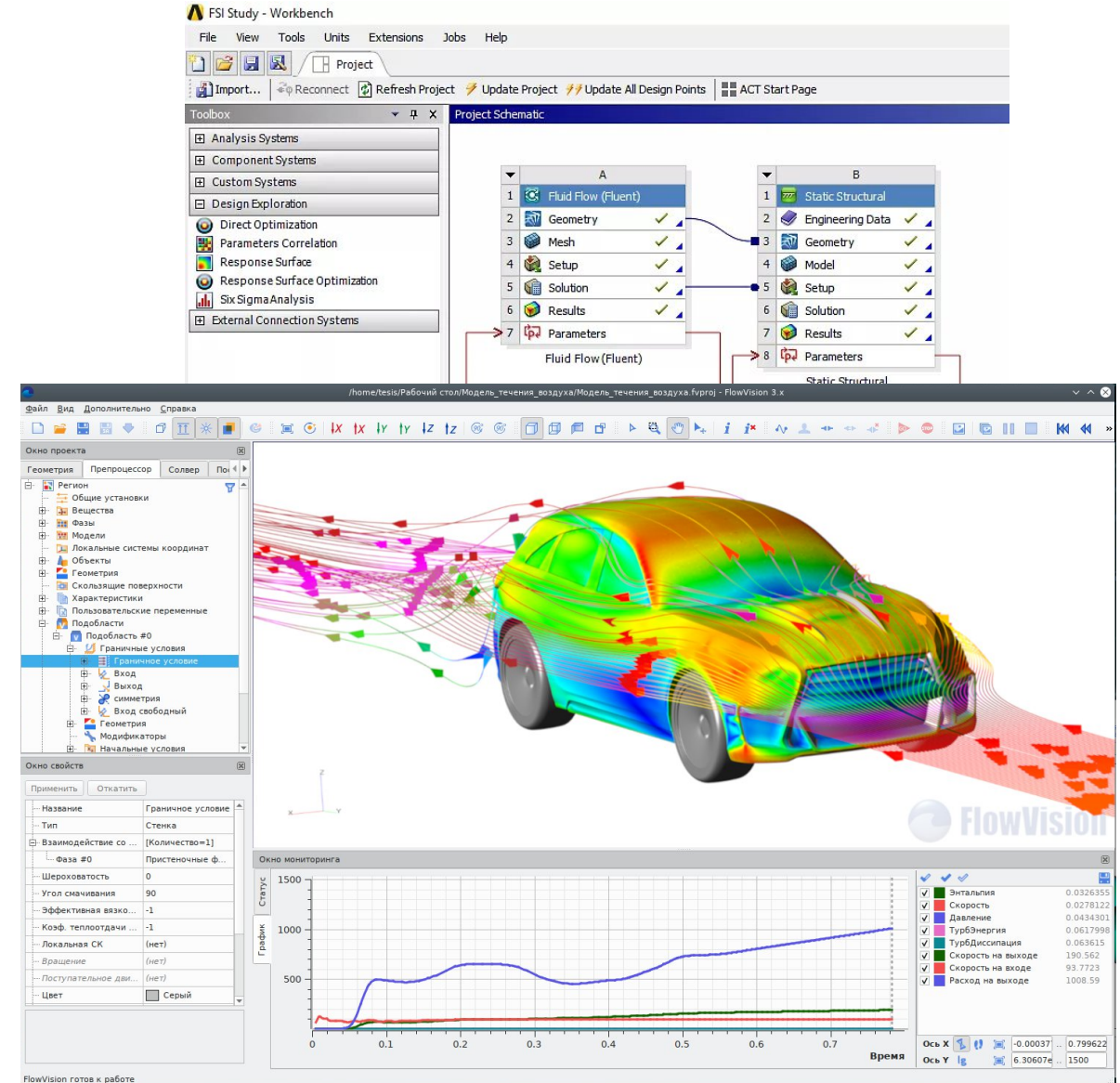
Relevance

- 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



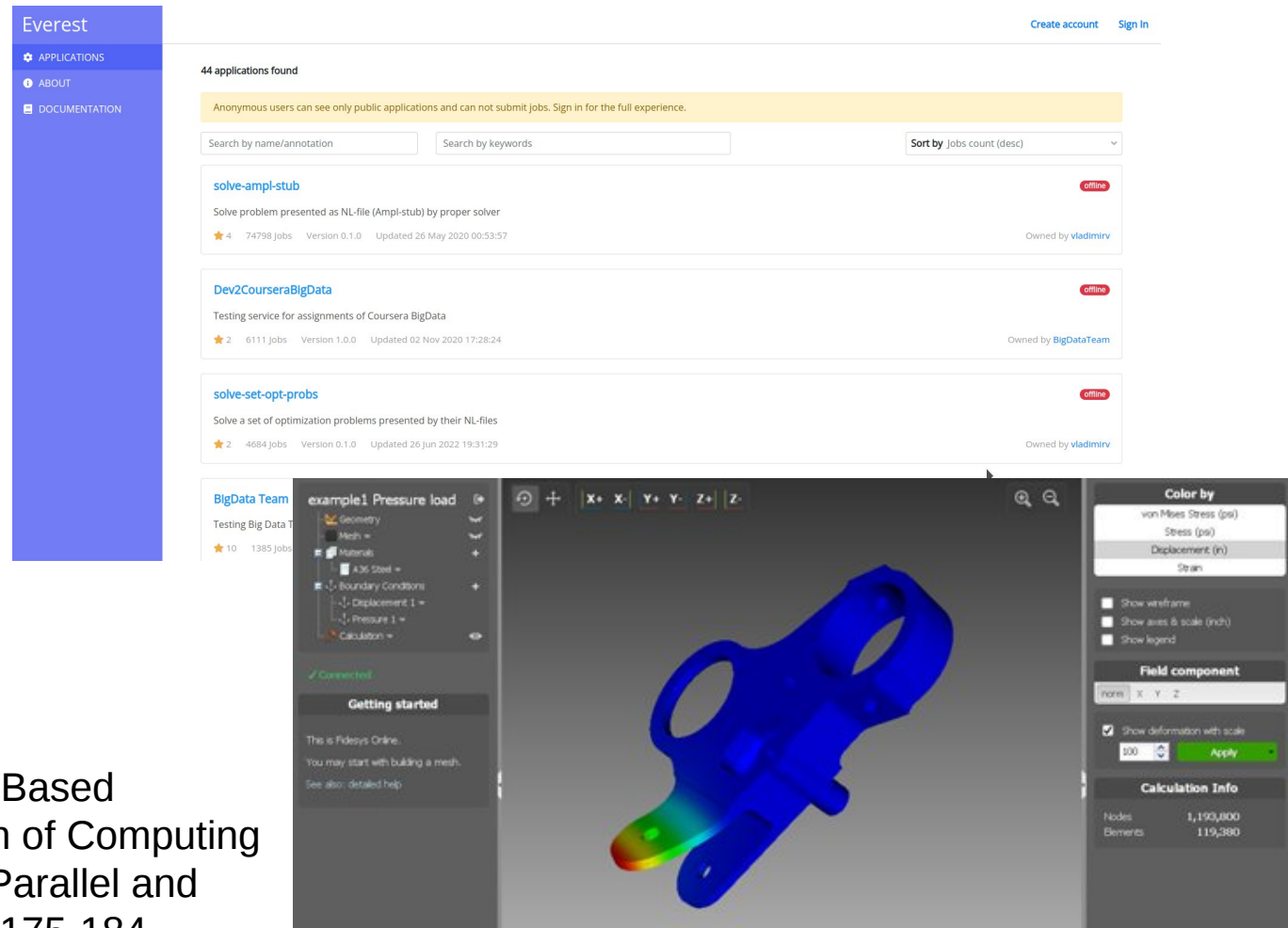
Web laboratories

- Domain specific web laboratories have a rich and responsive GUI^{1,2}
- Generalized web laboratories have ability to integrate third-party applications³

¹<https://www.sim4design.com>

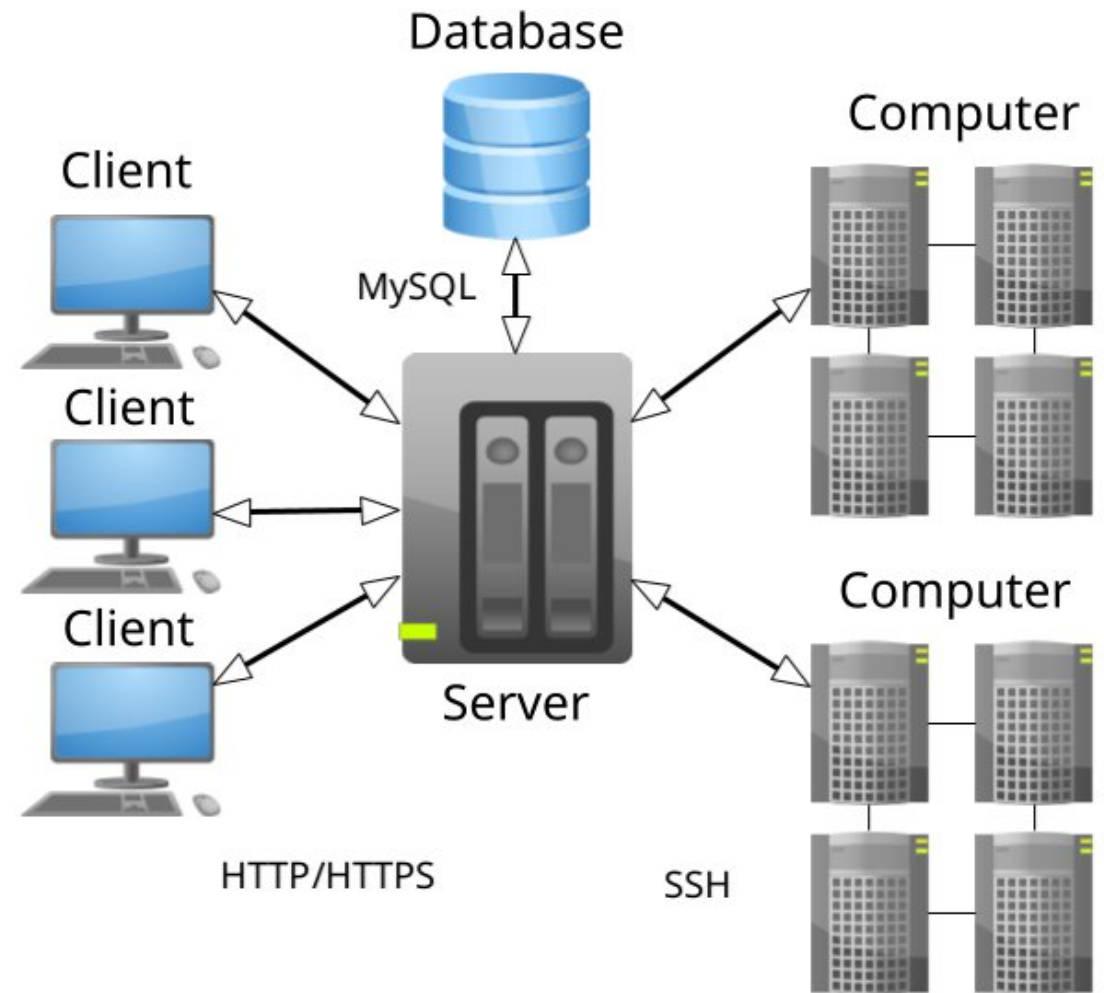
²<https://nucleonica.com/>

³Sukhoroslov 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:

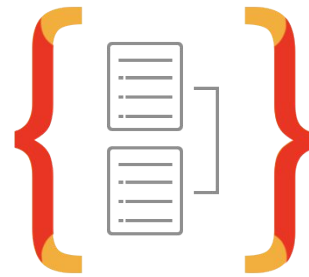
- TypeScript

Server:

- Node.js
- Express.js
- TypeORM

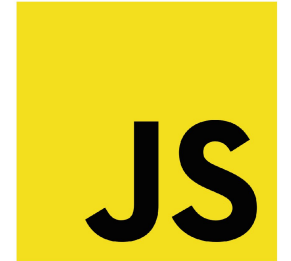
Client:

- Vue.js
- Quasar



TYPEORM

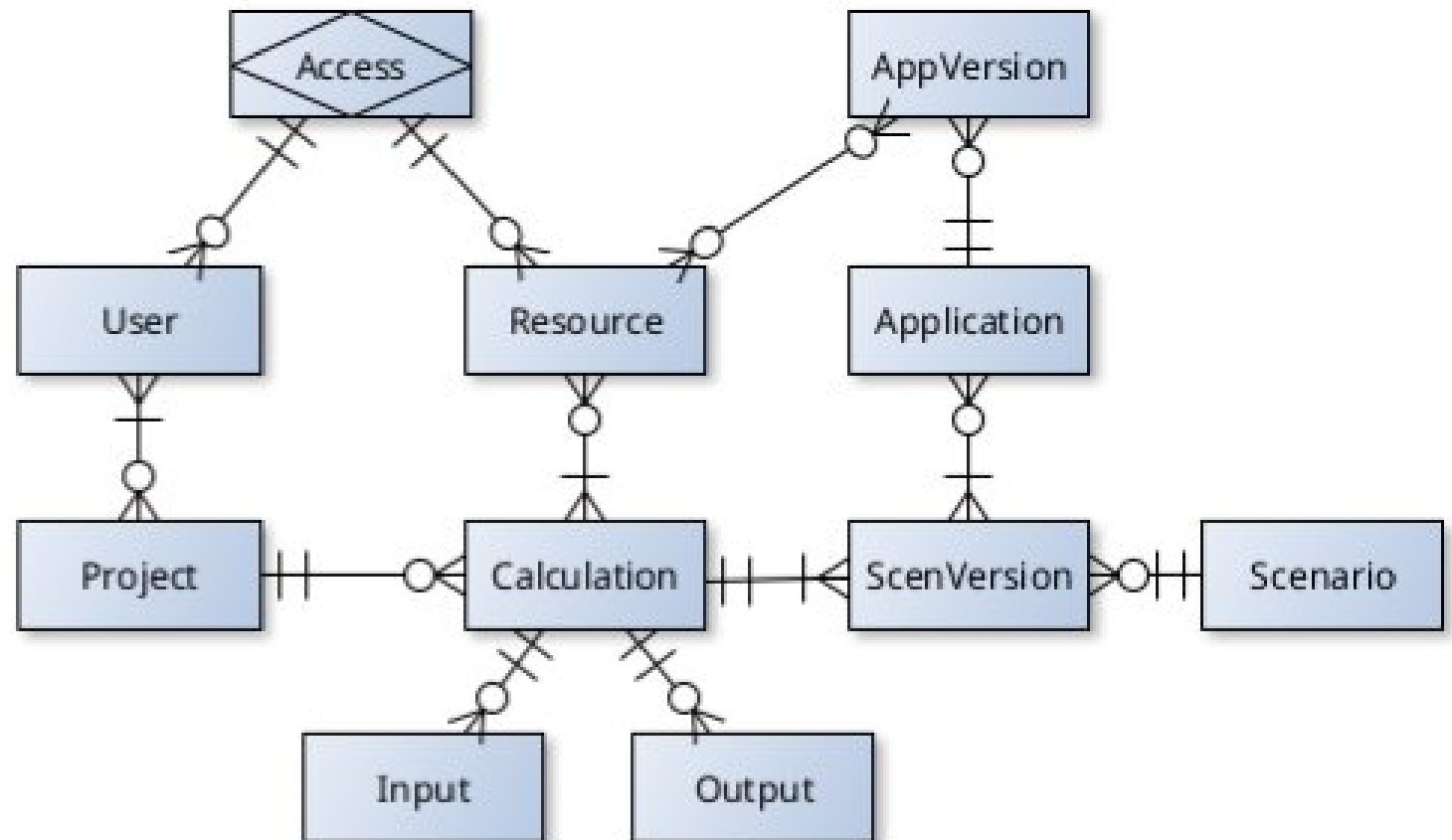
Express



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

Resources / New Record

New Resource

Name

Example

Access Type

ssh

Address

127.0.0.1

Port

22

Queue System

native

Environment

Resources / Resource

Resource Example

Address: localhost:22

Queue System: native

Access

USER NAME

TERMINAL

SHOW SSH-RSA

User Name: nikita

Working Directory: /home/nikita/WorkDir

Status: success

Application

DEPLOY

Name	Version	Action	Status	Streams
Solver	Solver V2	build	success	STDOUT STDERR

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

The screenshot displays two overlapping windows from a web application. The top window, titled 'Scenarios / Scenario / New Record', shows a 'Script' editor with the following YAML content:

```
1 applications:
2   hgSolver: hgSolver
3 connections: []
4 stages:
5   - run(hgSolver)
```

A 'CHECK' button is visible above the script editor. The bottom window, titled 'Applications / Application / New Record', shows a 'Passport' editor with the following YAML content:

```
1 build:
2   mkdir build; cd build; cmake ../; make -j4
3 exec:
4   comm: build/solver config.json
5 runBy:
6   type: exec
7 inputs:
8   - type: file
9     ident: mesh
10    name: Mesh file
11    descr: Mesh file in inner format
12    options:
13      format: data
14      path: mesh.txt
15   - type: file
16     ident: jsoncfg
17     name: Configuration
18     descr: Configuration file in json format
19     options:
20       format: tabs
21       vertical: true
22       fType: json
23       path: config1.json
24   childs:
25     - type: category
26       ident: main
27       name: Main
28       descr: Main global parameters
29       options:
30         format: form
31       childs:
```

At the bottom of the interface, a 'Source Code' section shows a status bar with a checkmark and '897.0B / 100.00%'. Below this, a file named 'string.zip' is listed with the same size and a checkmark.

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

The image displays three overlapping screenshots of a web application interface, likely for project management and calculation configuration. The interface features a blue header bar with navigation icons and a user profile icon labeled 'UU'. The main content area is divided into sections for project management and calculation configuration.

Top Screenshot: Shows a navigation bar with 'Projects / Project / Calculation' and a dropdown menu. Below it, a table lists calculations with columns: DESCRIPTION, RESOURCE, INPUTS, RUN, and OUTPUTS. The first row shows 'Calculation First Calculation' with resource 'hgSolver' and user 'nikita@Example'.

Middle Screenshot: Shows a sidebar with tabs: MESH FILE, CONFIGURATION, and OUTCHECK. The 'MESH FILE' tab is active, displaying 'Upload' and 'Connect' buttons. Below, it shows 'File: workDir/projects/1/calc_1/finp' and a progress bar for 'Mesh file' at '0.0B / 0.00%'.

Bottom Screenshot: Shows a configuration form for 'Calculation First Calculation'. The form has tabs: DESCRIPTION, RESOURCE, INPUTS, RUN, and OUTPUTS. The 'INPUTS' tab is active, showing configuration parameters for 'HGSOLVER':

- MAIN: Solver Dim (2d)
- MESH: (empty)
- SOLVERS: Epsilon (0.000001)
- SOLUTION: Threads (4)

An 'ACCEPT' button is visible at the bottom right.

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

The screenshot displays a web-based interface for managing computer experiments. The top navigation bar is blue and contains a menu icon, the text "Projects / Project / Calculation", a bell icon, a chat icon, and a user profile icon labeled "UU". Below the navigation bar, the main content area shows the title "Calculation First Calculation" followed by a vertical ellipsis. The interface is divided into several sections:

- DESCRIPTION**: A table with columns "Pseudoname" and "Parameters". It lists "hgSolver".
- RESOURCE**: A table with columns "Stage" and "Status". It lists "run(hgSolver)" with status "hgSolver: done".
- INPUTS**: A table with columns "Streams", "STDOUT", and "STDERR". It lists "hgSolver".
- OUTPUTS**: A table with columns "Streams", "STDOUT", and "STDERR". It lists "hgSolver".

Below the main content area, there is a window titled "hgSolver: stdout" with a close button. This window displays a log of the experiment's output, showing a series of steps and iterations with associated time and TAU values.

Step	Time	IterNb	TAU	CTime, ms
55	10.2325	16372	0.000625	862
56	10.4331	16693	0.000625	735
57	10.6337	17014	0.000625	819
58	10.8344	17335	0.000625	746
59	11.035	17656	0.000625	1081
60	11.2356	17977	0.000625	1025
61	11.4362	18298	0.000625	801
62	11.6369	18619	0.000625	689
63	11.8375	18940	0.000625	881
64	12.0381	19261	0.000625	724
65	12.2387	19582	0.000625	819
66	12.4394	19903	0.000625	909
67	12.64	20224	0.000625	747
68	12.8406	20545	0.000625	744
69	13.0412	20866	0.000625	769
70	13.2419	21187	0.000625	712
71	13.4425	21508	0.000625	776
72	13.6431	21829	0.000625	734
73	13.8437	22150	0.000625	728
74	14.0444	22471	0.000625	709
75	14.245	22792	0.000625	761
76	14.4456	23113	0.000625	818
77	14.6462	23434	0.000625	711
78	14.8469	23755	0.000625	720
79	15.0475	24076	0.000625	1010
80	15.2481	24397	0.000625	741
81	15.4487	24718	0.000625	793
82	15.6494	25039	0.000625	748
83	15.85	25360	0.000625	785
84	16.0506	25681	0.000625	838

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

The screenshot displays a web application interface for numerical results analysis. The top navigation bar shows the path "Projects / Project / Calculation" and includes a search icon, a notification bell, and a user profile icon labeled "UU".

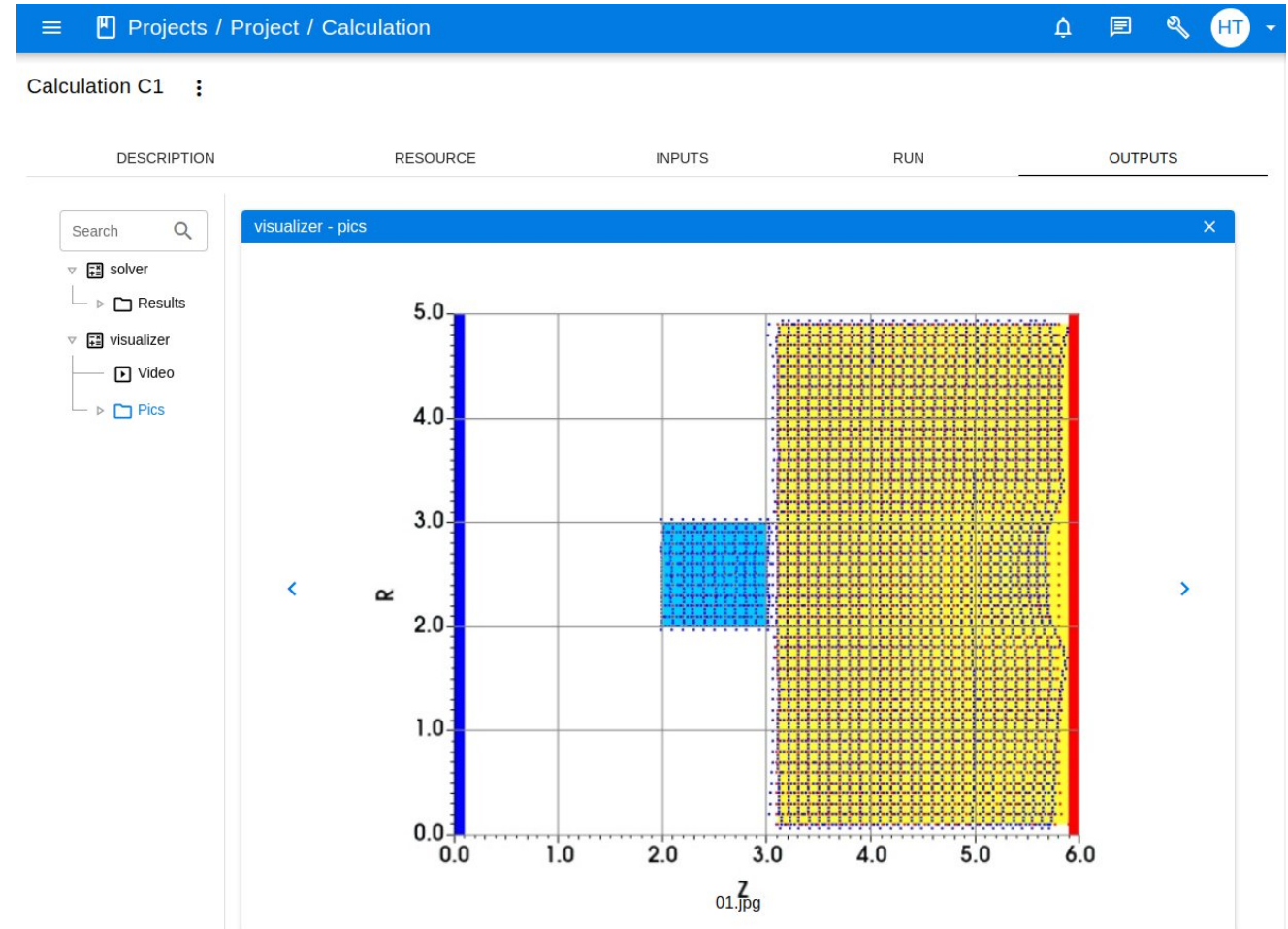
The main content area is divided into two sections. The left section, titled "Calculation First Calculation", shows a file explorer view with a search bar and a tree structure containing "hgSolver", "VisDir", and "DataFile". The right section, also titled "Calculation First Calculation", displays a table with columns: DESCRIPTION, RESOURCE, INPUTS, RUN, and OUTPUTS.

The table content is as follows:

DESCRIPTION	RESOURCE	INPUTS	RUN	OUTPUTS
hgSolver - test.txt				
31 Step: 28	Time: 5.40865	IterNb: 9586	TAU: 0.000564224	CTime, ms: 6306
32 Step: 29	Time: 5.60895	IterNb: 9941	TAU: 0.000564224	CTime, ms: 5654
33 Step: 30	Time: 5.80925	IterNb: 10296	TAU: 0.000564224	CTime, ms: 5518
34 Step: 31	Time: 6.00955	IterNb: 10651	TAU: 0.000564224	CTime, ms: 5595
35 Step: 32	Time: 6.20985	IterNb: 11006	TAU: 0.000564224	CTime, ms: 5382
36 Step: 33	Time: 6.41015	IterNb: 11361	TAU: 0.000564224	CTime, ms: 5065
37 Step: 34	Time: 6.61045	IterNb: 11716	TAU: 0.000564224	CTime, ms: 5641
38 Step: 35	Time: 6.81075	IterNb: 12071	TAU: 0.000564224	CTime, ms: 5922
39 Step: 36	Time: 7.01105	IterNb: 12426	TAU: 0.000564224	CTime, ms: 5363
40 Step: 37	Time: 7.21135	IterNb: 12781	TAU: 0.000564224	CTime, ms: 6059
41 Step: 38	Time: 7.41165	IterNb: 13136	TAU: 0.000564224	CTime, ms: 5682
42 Step: 39	Time: 7.61195	IterNb: 13491	TAU: 0.000564224	CTime, ms: 5290
43 Step: 40	Time: 7.81225	IterNb: 13846	TAU: 0.000564224	CTime, ms: 5632
44 Step: 41	Time: 8.01255	IterNb: 14201	TAU: 0.000564224	CTime, ms: 5845
45 Step: 42	Time: 8.21285	IterNb: 14556	TAU: 0.000564224	CTime, ms: 5979
46 Step: 43	Time: 8.41315	IterNb: 14911	TAU: 0.000564224	CTime, ms: 5895
47 Step: 44	Time: 8.61344	IterNb: 15266	TAU: 0.000564224	CTime, ms: 5757
48 Step: 45	Time: 8.81374	IterNb: 15621	TAU: 0.000564224	CTime, ms: 5468
49 Step: 46	Time: 9.01404	IterNb: 15976	TAU: 0.000564224	CTime, ms: 5651
50 Step: 47	Time: 9.21434	IterNb: 16331	TAU: 0.000564224	CTime, ms: 6279
51 Step: 48	Time: 9.41464	IterNb: 16686	TAU: 0.000564224	CTime, ms: 5952
52 Step: 49	Time: 9.61494	IterNb: 17041	TAU: 0.000564224	CTime, ms: 6252
53 Step: 50	Time: 9.81524	IterNb: 17396	TAU: 0.000564224	CTime, ms: 6067
54 Step: 51	Time: 10.0155	IterNb: 17751	TAU: 0.000564224	CTime, ms: 5813
55 Step: 52	Time: 10.2158	IterNb: 18106	TAU: 0.000564224	CTime, ms: 6499
56 Step: 53	Time: 10.4161	IterNb: 18461	TAU: 0.000564224	CTime, ms: 6082
57 Step: 54	Time: 10.6164	IterNb: 18816	TAU: 0.000564224	CTime, ms: 6126

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



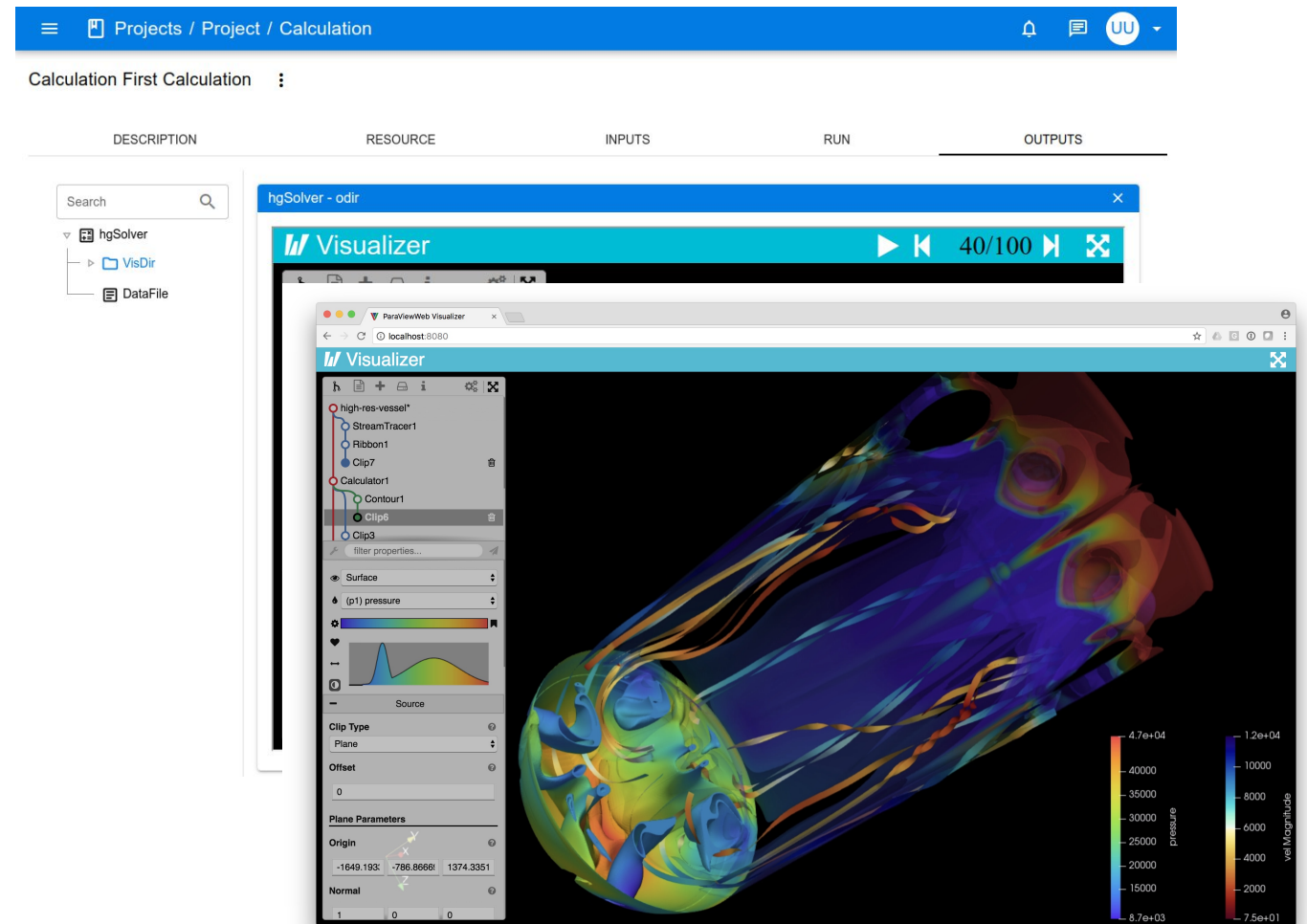
Interactive visualization

- Direct interactive visualization of data files. It is possible to use the following approaches:

- Embedding of Kitware Visualizer¹
- Developing original GUI to ParaViewWeb server²

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

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Thank you for your attention!