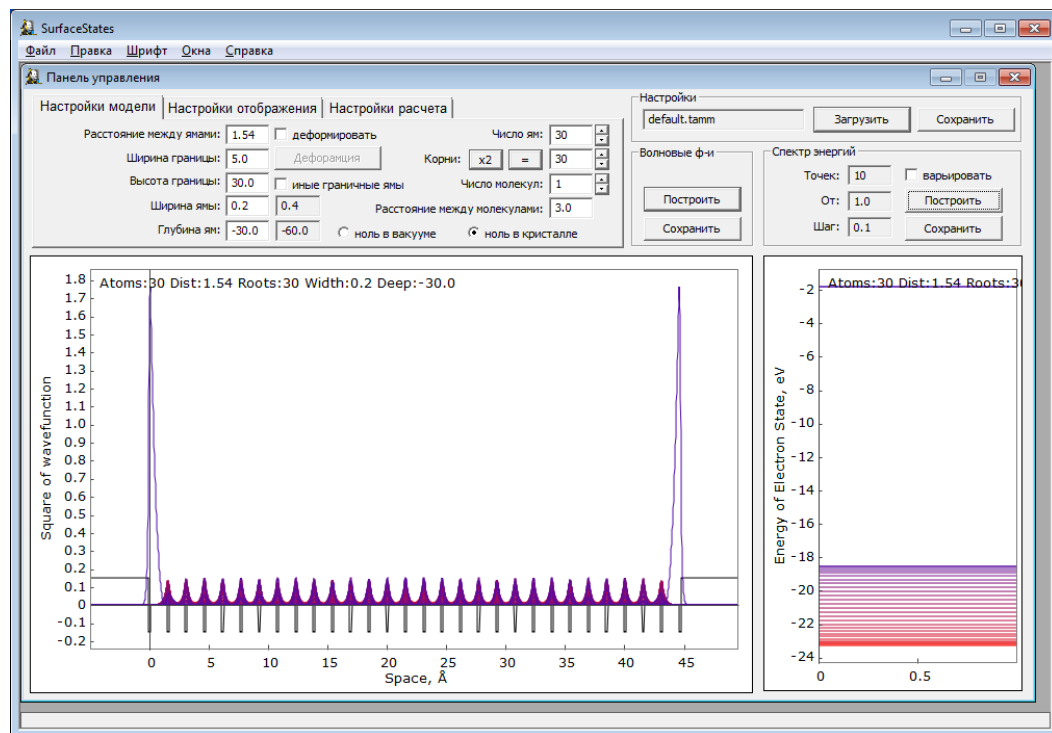
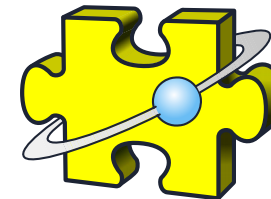


# Блэкбокс для компьютерного моделирования и 3D-визуализации

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# Графики



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## Nanodiamond Collective Electron States and their Localization

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The collective states despite their importance are rarely used to describe the electron structure of dielectric materials. The nature of the unrelated to impurities unpaired spins found experimentally in the nanodiamond is still under discussion. We propose the explanation of their nature in terms of the collective electron states. Collective states are studied by solving a one-particle one-dimensional Schrödinger equation in the Krönig-Penney potential and by *ab initio* computations of ground state wavefunctions of diamondoids  $C_{10}H_{14}$ ,  $C_{22}H_{30}$  and  $C_{54}H_{70}$  at the DFT R-B3LYP/6-31G(d,p) level of theory. Three distinct classes were found: collective bonding states resembling modulated particle in a box solutions; surface-localized non-bonding conductive Tamm states and subsurface-localized bonding states for non-uniformly compressed nanodiamond. The existence of the unpaired spins is supposed to result from the spin-density fluctuation effects significant on the nanoscale collective and spread subsurface states.

**Keywords:** nanodiamond, nanoscale, collective electron states, Tamm states, subsurface electron states, nanodiamond paramagnetism, spin-density fluctuations.

## Introduction

Collective electron states are widely used in the theory of metals [1], while bulk dielectric and semiconductor materials are equally well modeled as a rigid network of covalent bonds incorporating lattice defects. Success for classic models is mainly due to extensive use of translational symmetry, which is definitely not the case for nano-sized systems: nanoparticles are mostly imperfections with perfect regions rather than perfect crystals with imperfections. Lattice termination is the main imperfection leading to the consideration of the collective surface-localized

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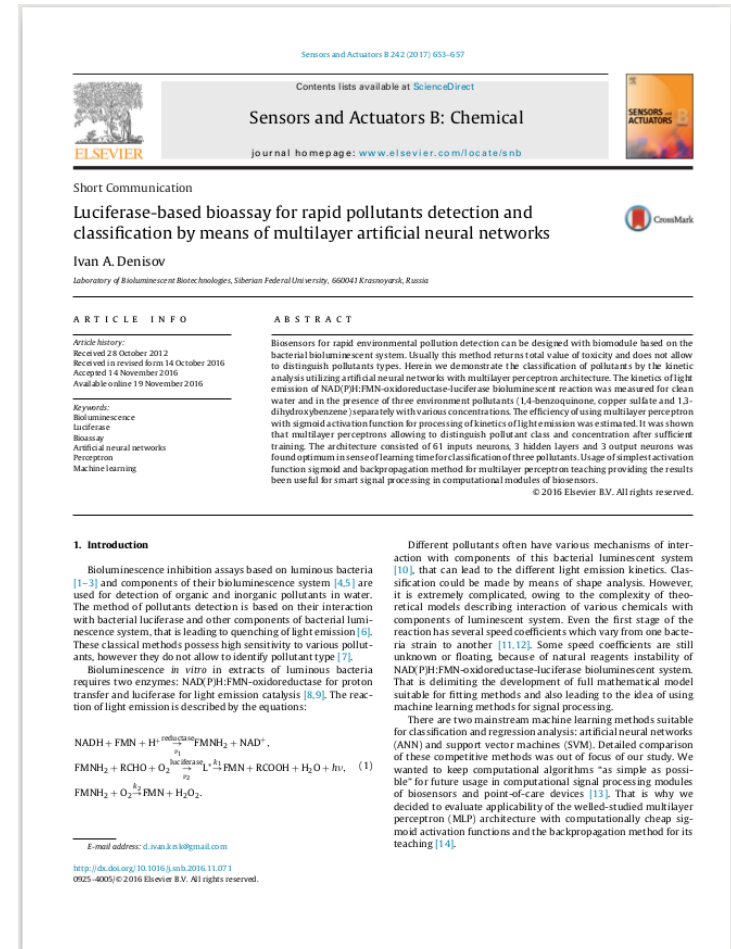
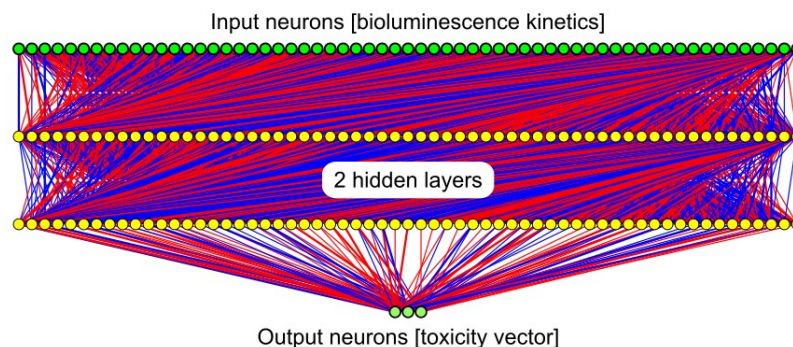
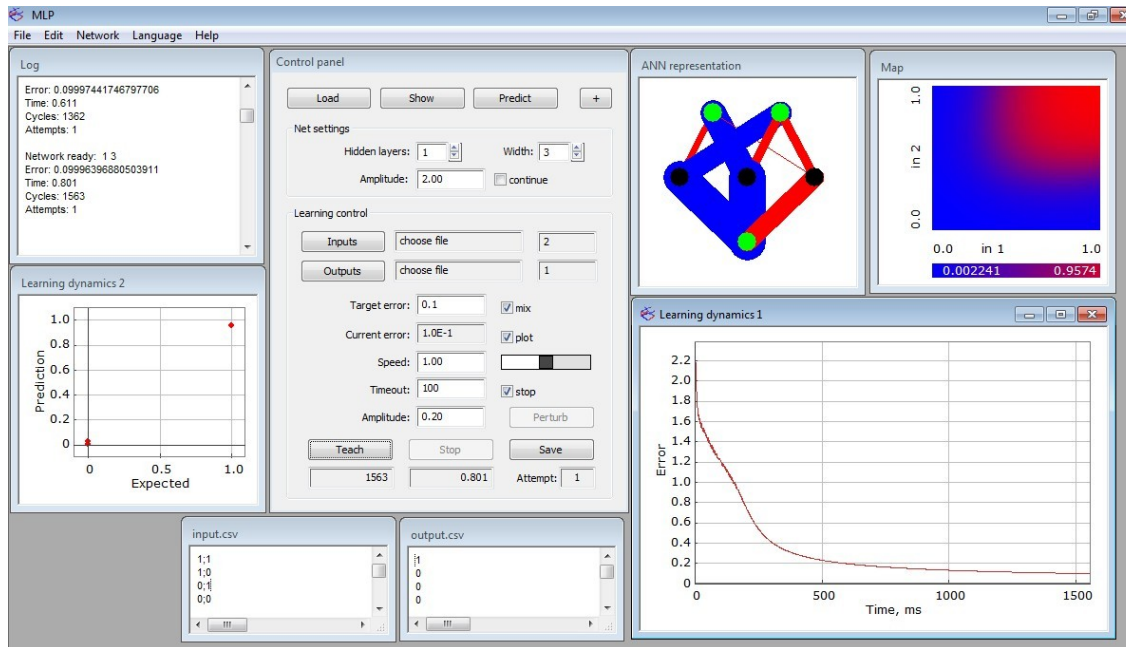
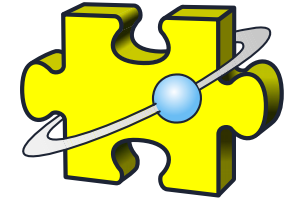
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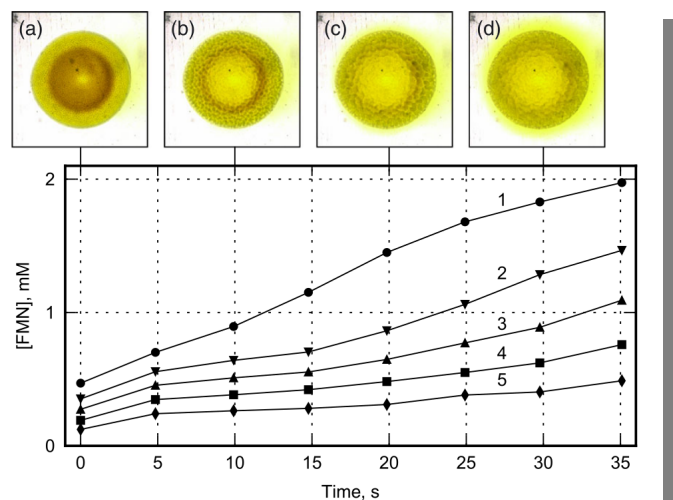
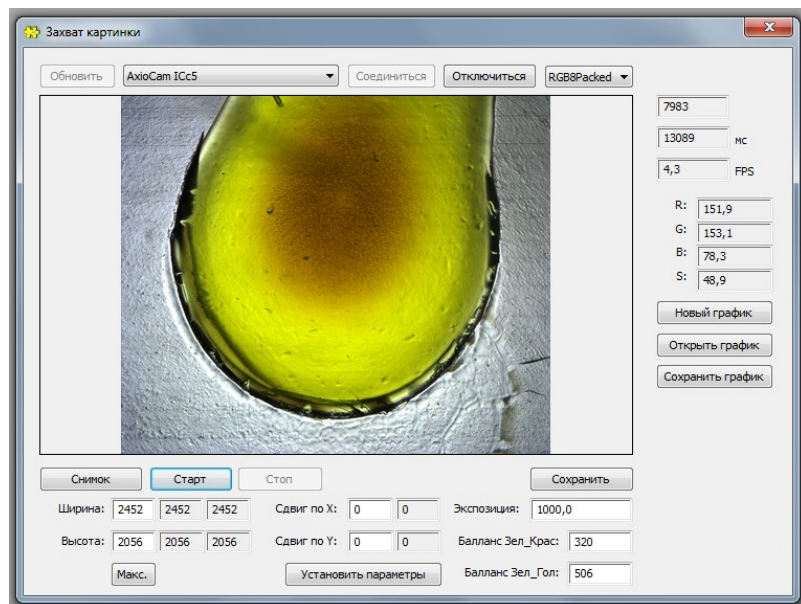
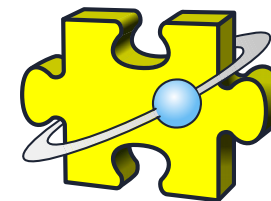
# Искусственные нейронные сети в Блэкбоксе



DOI: 10.1016/j.snb.2016.11.071



# Анализ изображений



Received: 22 November 2017 | Revised: 22 April 2018 | Accepted: 30 April 2018  
DOI: 10.1002/bio.3508

## RESEARCH ARTICLE

WILEY **LUMINESCENCE**  
The Journal of Biological and Chemical Luminescence

### Disposable luciferase-based microfluidic chip for rapid assay of water pollution

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#### Abstract

In the present study, we demonstrate the use of a disposable luciferase-based microfluidic bioassay chip for environmental monitoring and methods for fabrication. The designed microfluidic system includes a chamber with immobilized enzymes of bioluminescent bacteria *Photobacterium leiognathi* and *Vibrio fischeri* and their substrates, which dissolve after the introduction of the water sample and thus activate bioluminescent reactions. Limits of detection for copper (II) sulfate, 1,3-dihydroxybenzene and 1,4-benzoquinone for the proposed microfluidic biosensor measured 3  $\mu$ M, 15  $\mu$ M, and 2  $\mu$ M respectively, and these values are higher or close to the level of conventional environmental biosensors based on lyophilized bacteria. Approaches for entrapment of enzymes on poly(methyl methacrylate) (PMMA) plates using a gelatin scaffold and solvent bonding of PMMA chip plates under room temperature were suggested. The proposed microfluidic system may be used with some available luminometers and future portable luminescence readers.

#### KEYWORDS

bioassay, lab-on-a-chip, luciferase, microfluidics, solvent bonding

## 1 | INTRODUCTION

Increasing human negative impact on water reservoirs<sup>[1]</sup> and soils<sup>[2,3]</sup> necessitate development of methods for environmental monitoring. Over the past 40 years, biosensors have emerged as promising tools for rapid pollutant detection in different samples.<sup>[4–6]</sup> One of the major trends is to design biosensors suitable for point-of-care testing (POCT),<sup>[7]</sup> which have been extensively developed in the last decade.<sup>[8,9]</sup> According to the POCT concept, assays should be performed on-site with the help of handheld devices.<sup>[10]</sup> Such devices offer cost-effective alternative to expensive and time-consuming laboratory tests.

Glucometers with plastic or paper strips represent the most known example of point-of-care (POC) devices.<sup>[11]</sup> Some of the POC

devices use special systems with several wells for bioluminescent bacteria sensors.<sup>[12]</sup> A standard microtiter plate can also be used for sample holding in POC devices.<sup>[13]</sup> There are POC electrochemical devices for lactate monitoring that use special patches from fibers.<sup>[14]</sup> Many POCT devices include built-in microfluidic chips, in which processes of sample preparation, fluid manipulation and detection are automated.<sup>[15–17]</sup>

Electrochemical biosensors are one of the most common and commercially successful types of POCT devices.<sup>[18,19]</sup> In recent years there has been a trend for using smartphones in POC diagnostics.<sup>[20,21]</sup> This is due to their high prevalence and the ability to easily connect peripheral sensors. Smartphones have become common tools for measuring the pulse<sup>[22]</sup> and they even can be used for cataract diagnostics.<sup>[23]</sup> However, the sensitivity of the camera in a smartphone limits their application for POC diagnostics.

Different types of biosensor detection systems can be used for the determination of pollutants in water samples; however, the most suitable are optical-based biosensors.<sup>[24–26]</sup> Optical-based biosensors

**Abbreviations used:** FMN, flavin mononucleotide; HSV, hue, saturation and value; IC<sub>50</sub>, concentration of pollutants causing system inhibition by 50%; LOD, limit of detection; NADH, nicotinamide adenine dinucleotide; PMMA, poly(methyl methacrylate); POCT, point-of-care testing.

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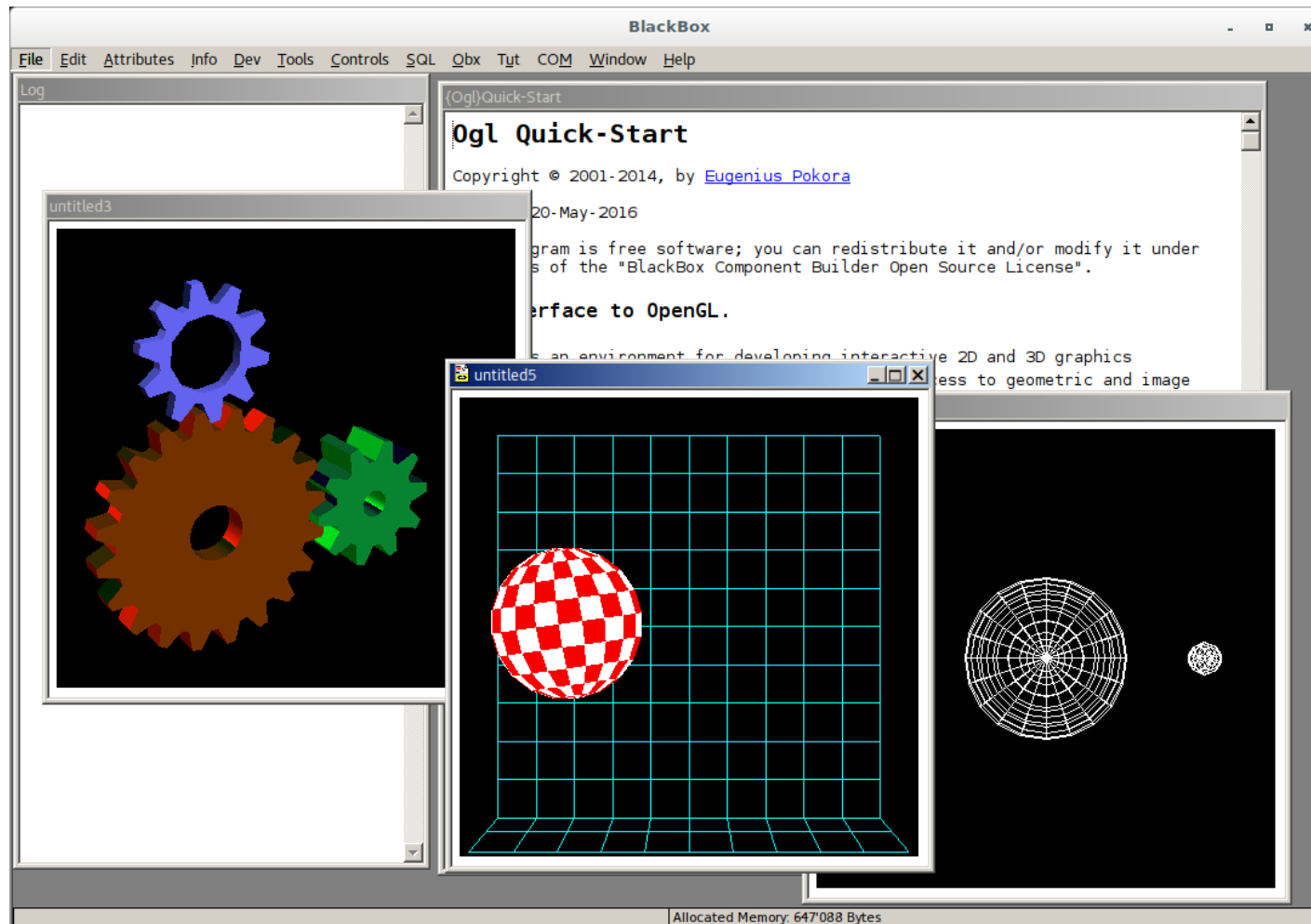
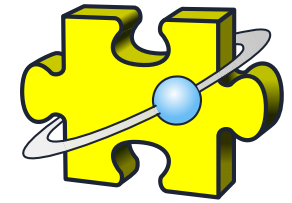
wileyonlinelibrary.com/journal/bio

Luminescence. 2018;33:1054–1061.

DOI: 10.1002/bio.3508



# Подсистема Ogl (Eugenius Pokora) Работает в новом Wine!

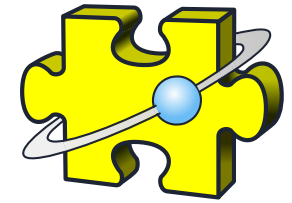




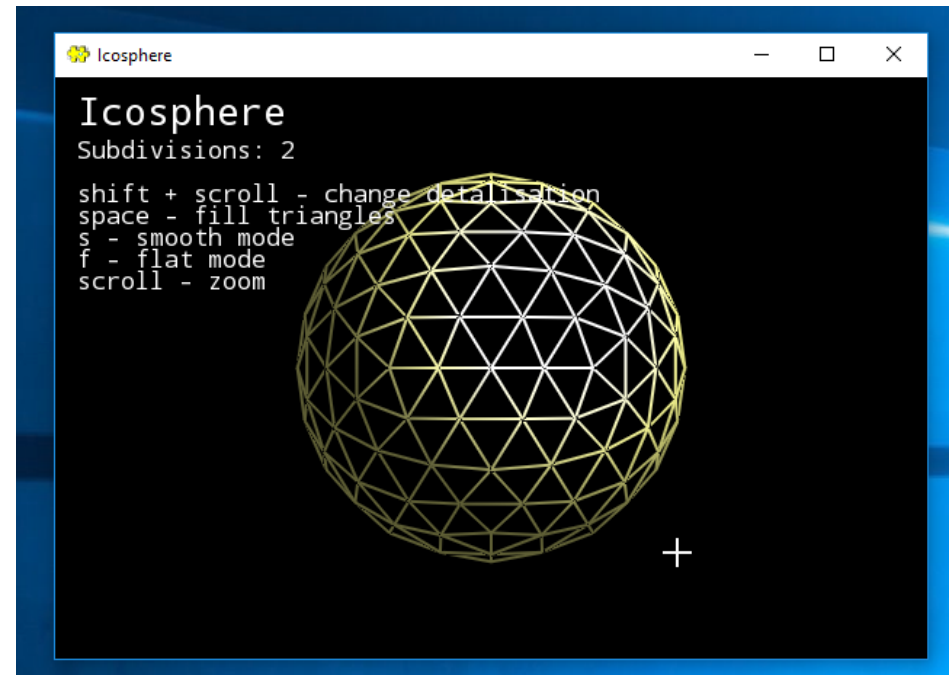
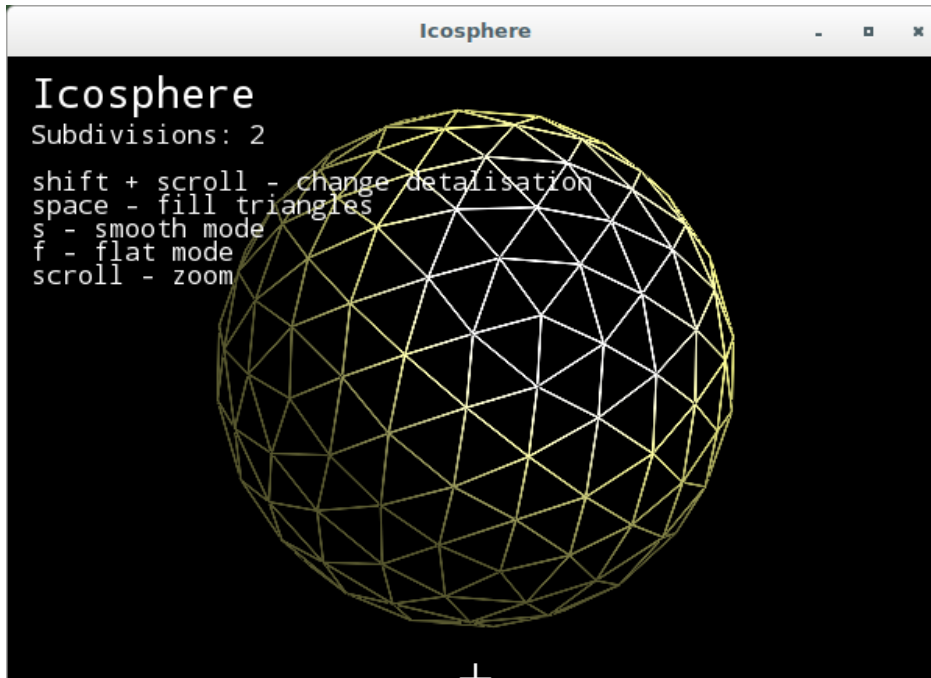


# SDL2 = Simple DirectMedia Layer

(П. Кушнир, И. Кузьмицкий, И. Денисов)



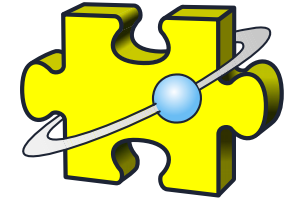
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# SDL2 = Simple DirectMedia Layer

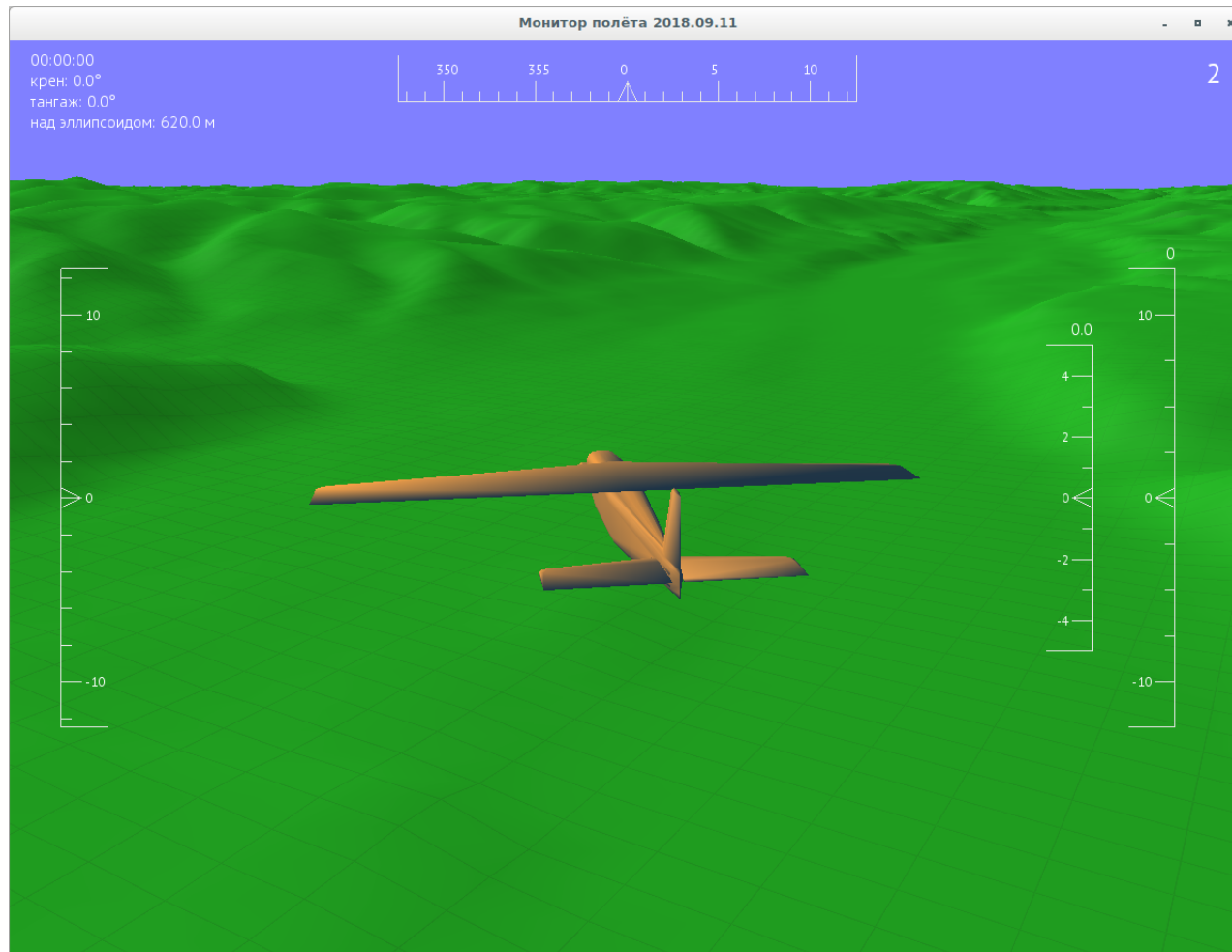
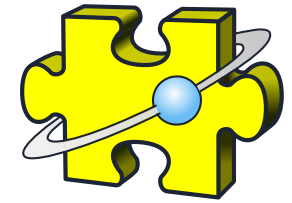
(П. Кушнир, И. Кузьмицкий, И. Денисов)



```
PROCEDURE Start*;
VAR res: INTEGER; updater: Update;
BEGIN
  (* Loading realisation of Sdl2Std abstract interface *)
  IF Dialog.IsWindows() THEN
    ASSERT(Kernel.ThisMod('Sdl2StdWin') # NIL, 20)
  ELSIF Dialog.IsLinux() THEN
    ASSERT(Kernel.ThisMod('Sdl2StdLin') # NIL, 20)
  ELSE
    HALT(20)
  END;
  width := initWidth;
  height := initHeight;
  res := Sdl2Lib.Init(Sdl2Const.INIT_VIDEO + Sdl2Const.INIT_EVENTS);
  w := Sdl2Video.CreateWindow("OpenGL window", 100, 100, width, height,
    Sdl2Const.WINDOW_OPENGL + Sdl2Const.WINDOW_RESIZABLE);
  c := Sdl2Video.GL_CreateContext(w);
  Sdl2Video.GL_MakeCurrent(w, c);
  Gl.ClearColor(0, 0, 0, 0);
  Gl.Enable(Gl.GL_COLOR_MATERIAL);
  Gl.ColorMaterial(Gl.GL_FRONT, Gl.GL_AMBIENT_AND_DIFFUSE);
  Viewport;
  NEW(loop);
  Sdl2Lib.StartLoop(loop);
  update:= FALSE;
  NEW(updater);
  Services.DoLater(updater, Services.now);
END Start;
```



# Проект «Монитор полета БЛА»

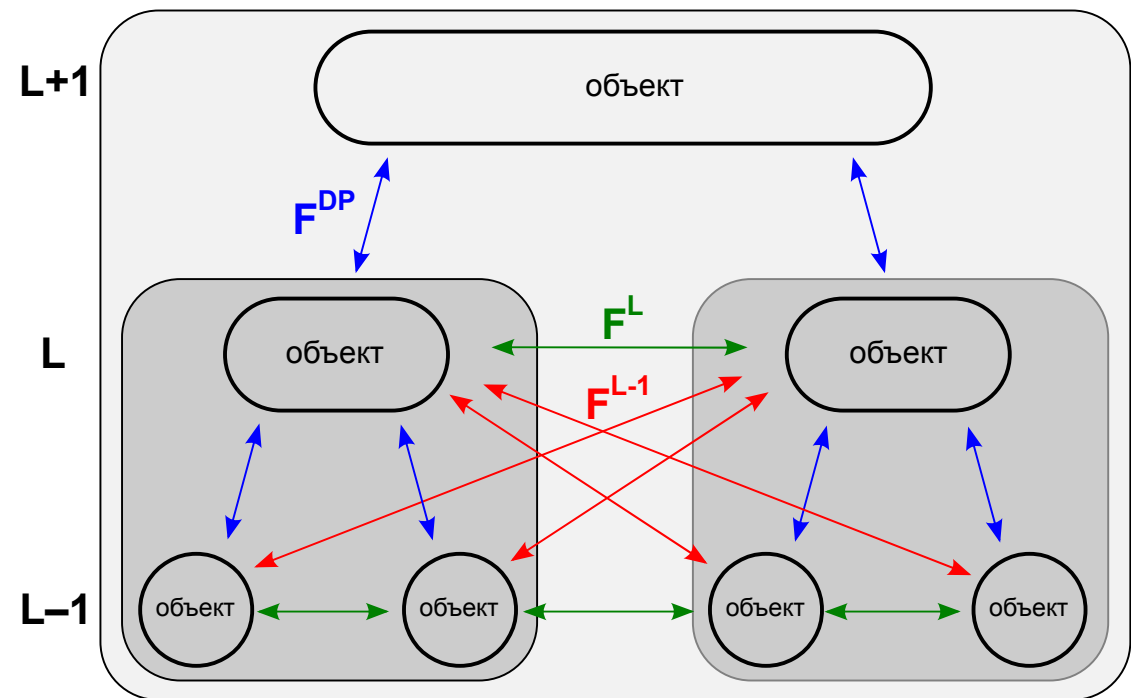
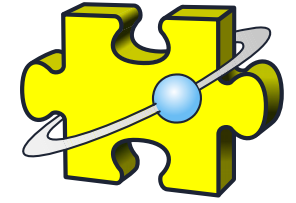


Визуализация ландшафта  
(**Shuttle Radar Topography Mission**)



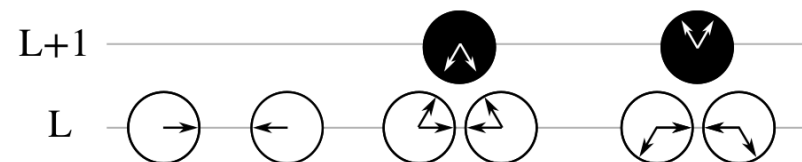
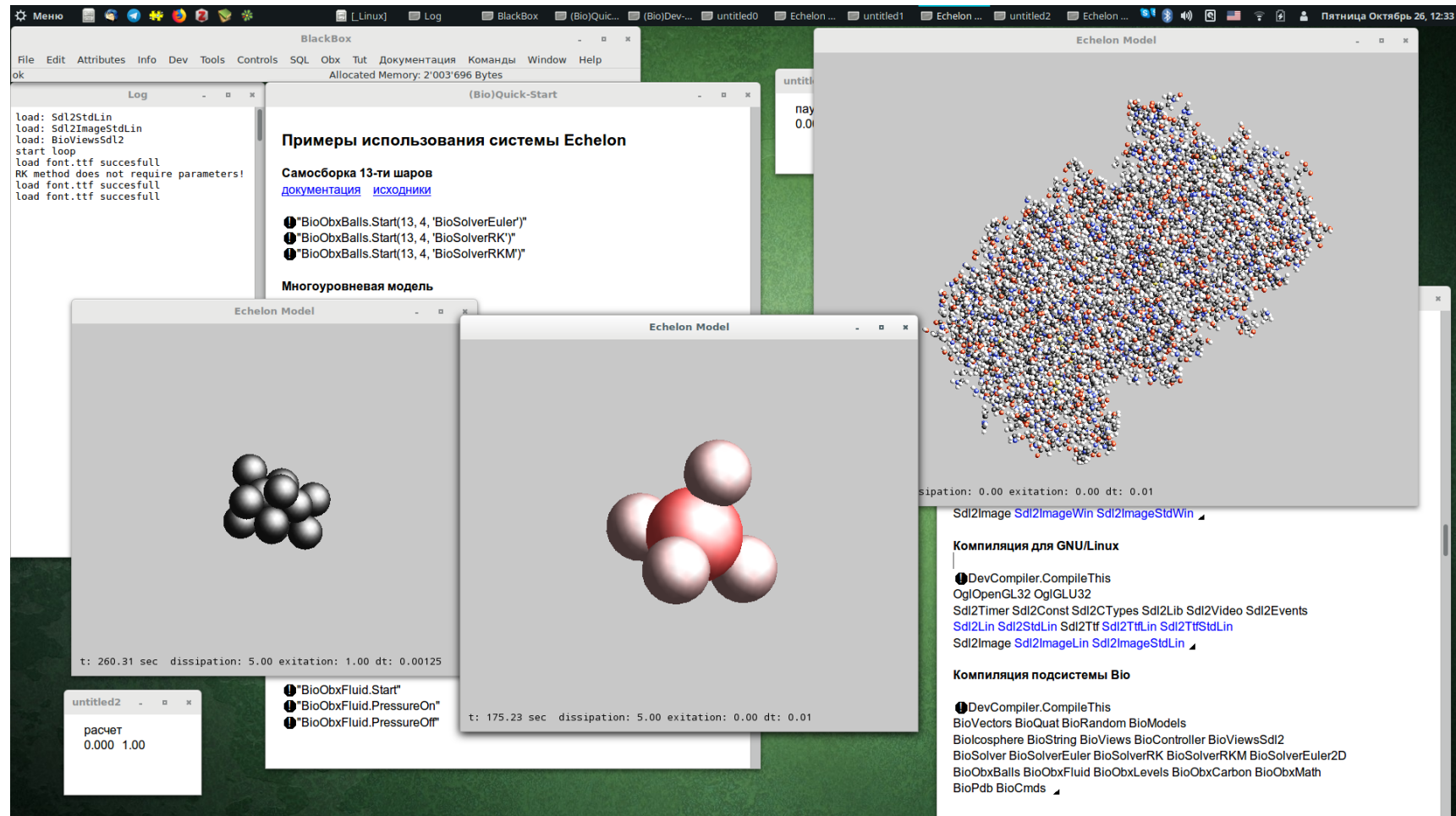
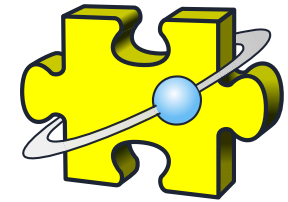


# Многоуровневое моделирование



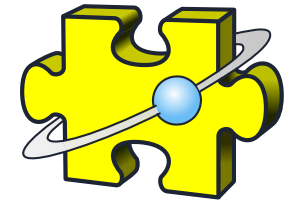


# Среда для моделирования ECHELON





# Подключение «солверов»



```
MODULE BioSolver;
```

```
IMPORT BioModels, BioVectors, Meta;
```

```
TYPE
```

```
  Force* = PROCEDURE(m: BioModels.Model; act: BioModels.Unit; OUT f: BioVectors.Vector);
```

```
  Solver* = POINTER TO ABSTRACT RECORD
```

```
    m*: BioModels.Model; (* модель *)
```

```
    f*: Force; (* сила *)
```

```
  END;
```

```
  Factory* = POINTER TO ABSTRACT RECORD END;
```

```
VAR factory: Factory;
```

```
PROCEDURE (d: Factory) New* (par: POINTER TO ARRAY OF REAL): Solver, NEW, ABSTRACT;
```

```
PROCEDURE (s: Solver) Step*, NEW, ABSTRACT;
```

```
PROCEDURE New* (par: POINTER TO ARRAY OF REAL): Solver;
```

```
BEGIN
```

```
  IF factory # NIL THEN RETURN factory.New(par) ELSE RETURN NIL END
```

```
END New;
```

```
PROCEDURE SetFactory* (d: Factory);
```

```
BEGIN factory := d
```

```
END SetFactory;
```

```
PROCEDURE Load* (solver: ARRAY OF CHAR): BOOLEAN;
```

```
VAR item: Meta.Item; proc: RECORD (Meta.Value) Install: PROCEDURE END; ok: BOOLEAN;
```

```
BEGIN
```

```
  Meta.LookupPath(solver + ".Install", item);
```

```
  IF item.Valid() & (item.obj = Meta.procObj) THEN
```

```
    item.GetVal(proc, ok);
```

```
    IF ok THEN proc.Install;
```

```
      RETURN TRUE END
```

```
  END;
```

```
  RETURN FALSE
```

```
END Load;
```

```
END BioSolver.
```

```
❗ "BioObxBalls.Start(13, 4, 'BioSolverEuler')"
```

```
❗ "BioObxBalls.Start(13, 4, 'BioSolverRK')"
```

```
❗ "BioObxBalls.Start(13, 4, 'BioSolverRKM')"
```