NEW PERSPECTIVES IN SCIENCE EDUCATION
16-19 March 2017, Florence, Italy

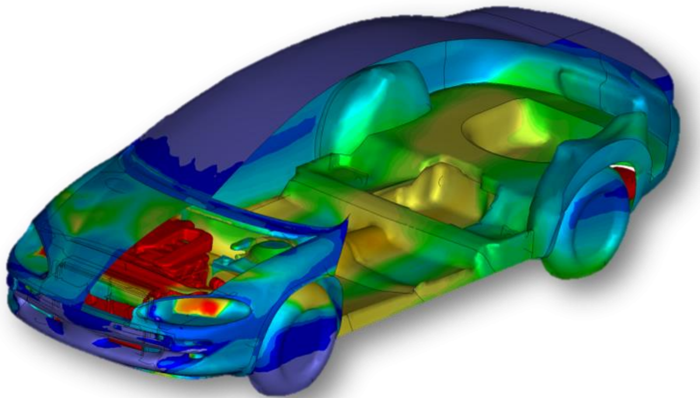
Usage FlexPDE Package in the Courses of Mathematical Modeling and Mechanics

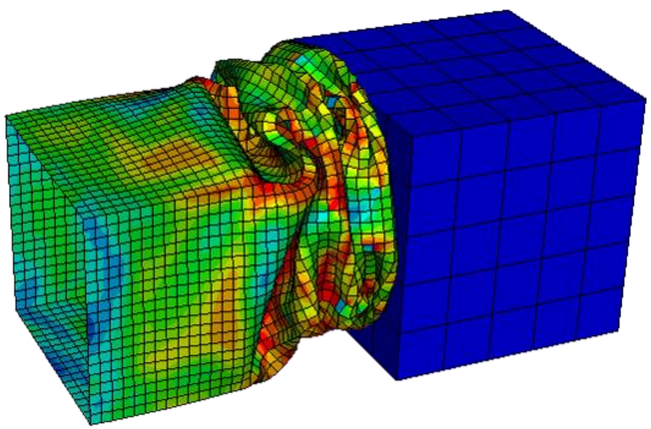
Olga Pustovalova, Mikhail Karyakin

I.I.Vorovich Institute of Mathematics, Mechanics and Computer Science
Southern Federal University, Rostov-on-Don, Russia

Contents

Well known Finite Element Packages





ANSYS®

ABAQUS

Superior Finite Element Analysis Solutions

MSC Nastran

Structural & Multidiscipline FEA

https://www.simuleon.com/simulia-abaqus/abaqus-explicit/
http://cae-expert.ru/product/ansys-cfx

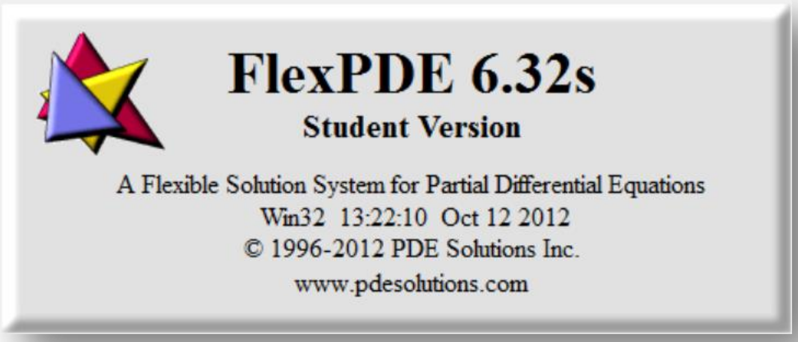
FlexPDE Package

Mechanics

Chemistry

Biology

Physics



Difference from other Packages

Ansys | Abaqus | Nastran

Geometry of Models → Mesh → Boundary Conditions → Numerical Analysis

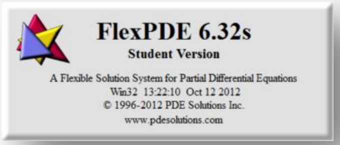
FlexPDE

Geometry of Models → Differential Equations and Boundary Conditions → Mesh → Numerical Analysis

Purposes and Possibilities

- **The Course involves solving educational tasks using finite element packages**

- **Using the finite element package FlexPDE allows to**
  - solve the problem described by differential equations in partial derivatives of the 1st and 2nd of orders
  - determine the geometry and boundary conditions
  - set accuracy of the solution
  - set output method results



Necessary Educational Background

- Differential equations
- Numerical methods
- Skills in Maple and MatLab packages
- Equations of mathematical physics
- Basics of theoretical mechanics
- Fundamentals of linear elasticity

Brief Program of Practical Training

- Stationary thermal conductivity
- Transient thermal conductivity
- Frequency analysis
- Determination of stress-strain state in the static problems of elasticity

Areas of science where we can apply FlexPDE

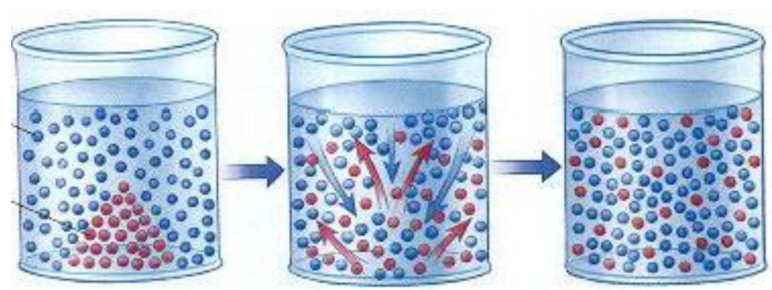
- Physics
- Mechanics
- Chemistry
- Biology

Planetary motion

Strain-Stress Solution

Reaction-diffusion

Microorganisms Colony Growth



The Problems described by the Poisson equation

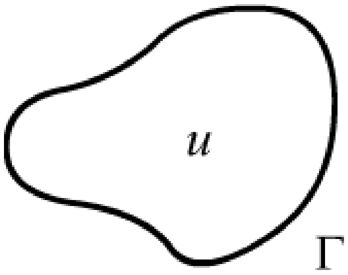
- Thermal conductivity
- Hydraulics
- Electrostatics
- Physics

Poisson's equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

$$u\big|_{\Gamma} = u_0$$

$$\left.\frac{\partial u}{\partial n}\right|_{\Gamma} = v_0$$

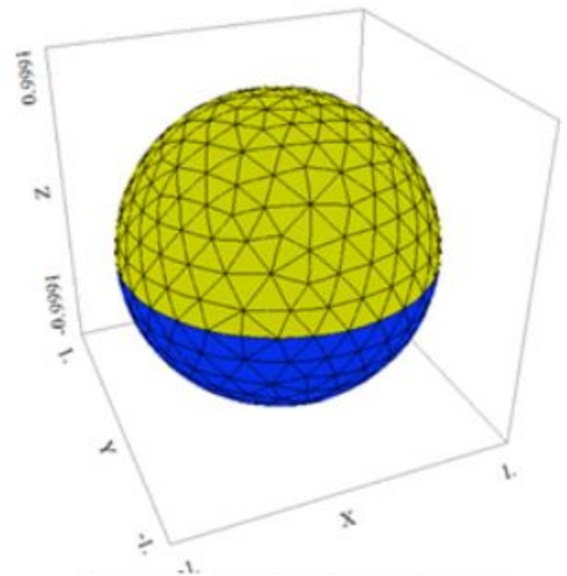


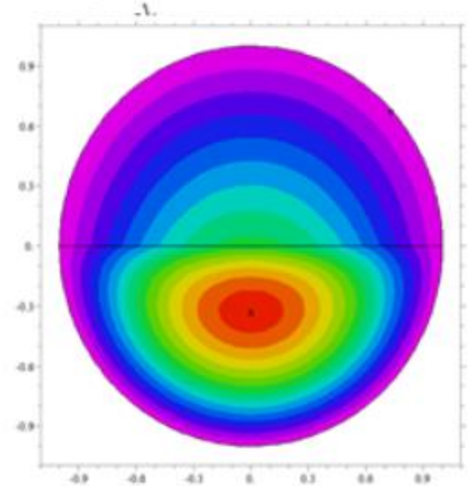
Main sections of FlexPDE script

TITLE	-	name of the task
COORDINATES	-	coordinate system
VARIABLES	-	variable of differential equations
DEFINITIONS	-	parameters of the problem
EQUATIONS	-	differential equations
BOUNDARIES	-	boundaries and boundary conditions
MONITORS	-	intermediate results
PLOTS	-	final results
END	-	end of program

The example of FlexPDE script

```
TITLE 'Stationary Heat Conductivity'
COORDINATES
    cartesian3
SELECT
painted
VARIABLES u
DEFINITIONS
    K = 0.1      { conductivity }
    R0 = 1       { radius }
    H0 = 100     { total heat }
    heat =H0*exp(-x^2-y^2-z^2) { volume heat source }
EQUATIONS
    div(K*grad(u)) + heat = 0
  extrusion
   surface z = -sqrt(R0^2 - (x^2+y^2))  { the bottom hemisphere }
   surface z=0
   surface z = sqrt(R0^2  -(x^2+y^2))   { the top hemisphere }
BOUNDARIES
    surface 1 value(u) = 0
    surface 3 value(u) = 0
    Region 1
      layer 1 K=0.1
      layer 2 K=0.5
      start  (R0,0)  arc(center=0,0) angle=360
PLOTS
    grid(x,y,z)
    contour(u) on x=0
END
```





Problems

Analytical solutions ⟷ Numerical solutions

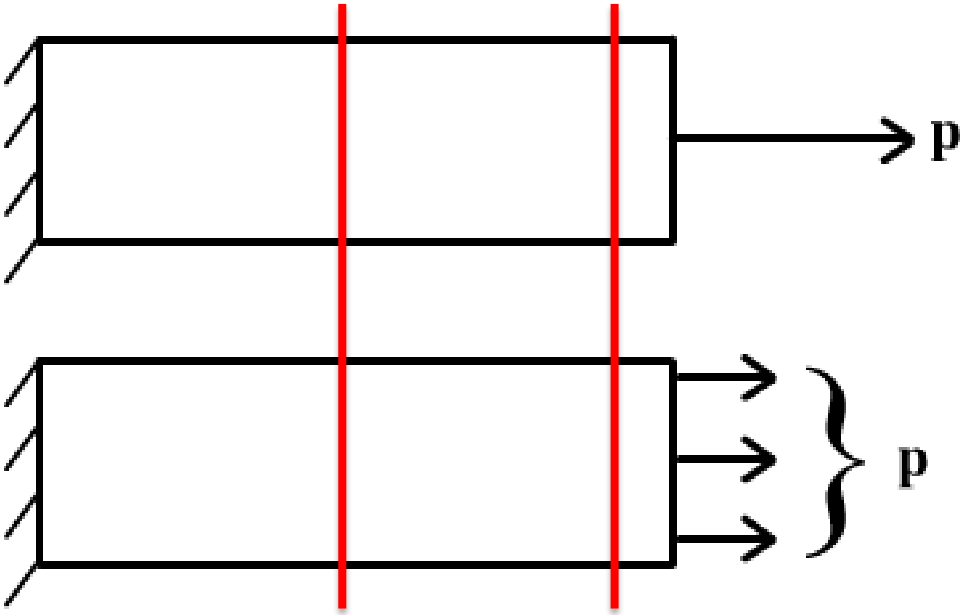
Examples

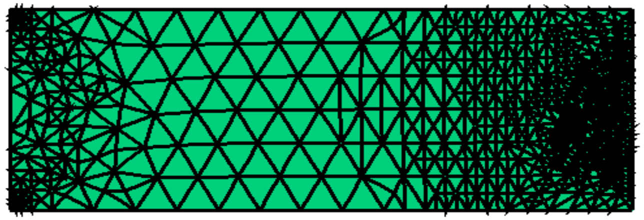
1. Saint-Venant's principle
2. Typical tasks for students:
   - ✓ The Kirsch problem
   - ✓ Frequency analysis

Example 1. Saint-Venant's principle

Near

Far away





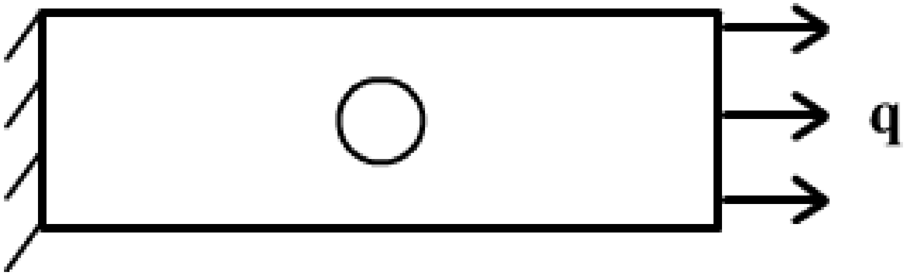
2D

3D

Example 2. The Kirsch problem

Tension of the Bar with a Hole

$$k = \frac{\sigma_{\max}}{\sigma_n}$$



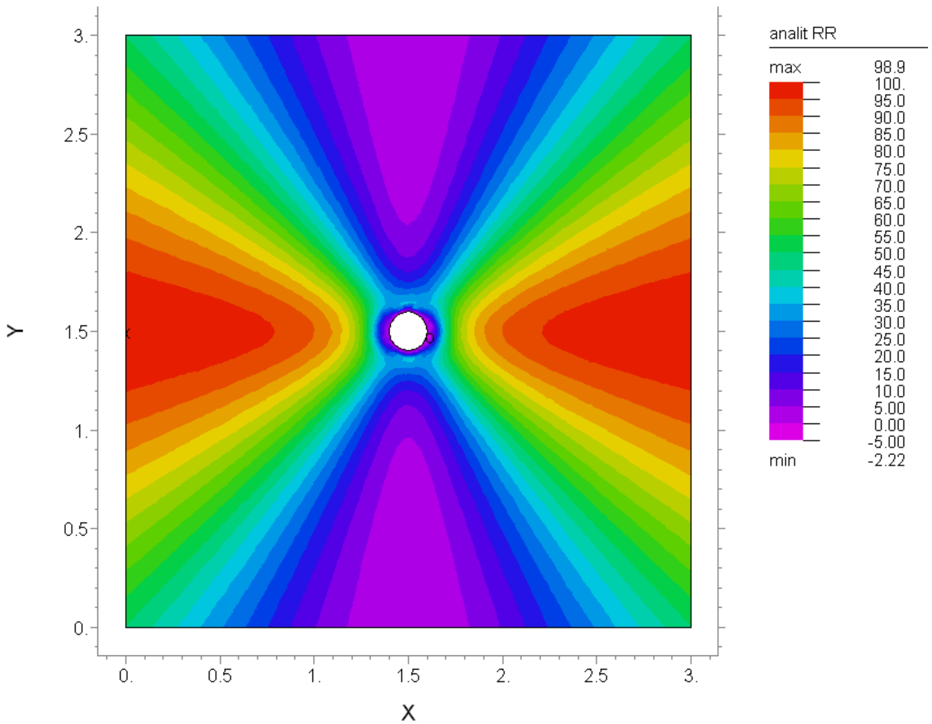
$$\sigma_{rr} = \frac{p}{2}\left(1 - \frac{R^2}{r^2}\right) + \frac{p}{2}\left(1 - \frac{4R^2}{r^2} + \frac{3R^4}{r^4}\right)\cos 2\varphi$$

$$\sigma_{\varphi\varphi} = \frac{p}{2}\left(1 + \frac{R^2}{r^2}\right) - \frac{p}{2}\left(1 - \frac{3R^4}{r^4}\right)\cos 2\varphi$$

$$\sigma_{r\varphi} = -\frac{p}{2}\left(1 + \frac{2R^2}{r^2} - \frac{3R^4}{r^4}\right)\sin 2\varphi$$

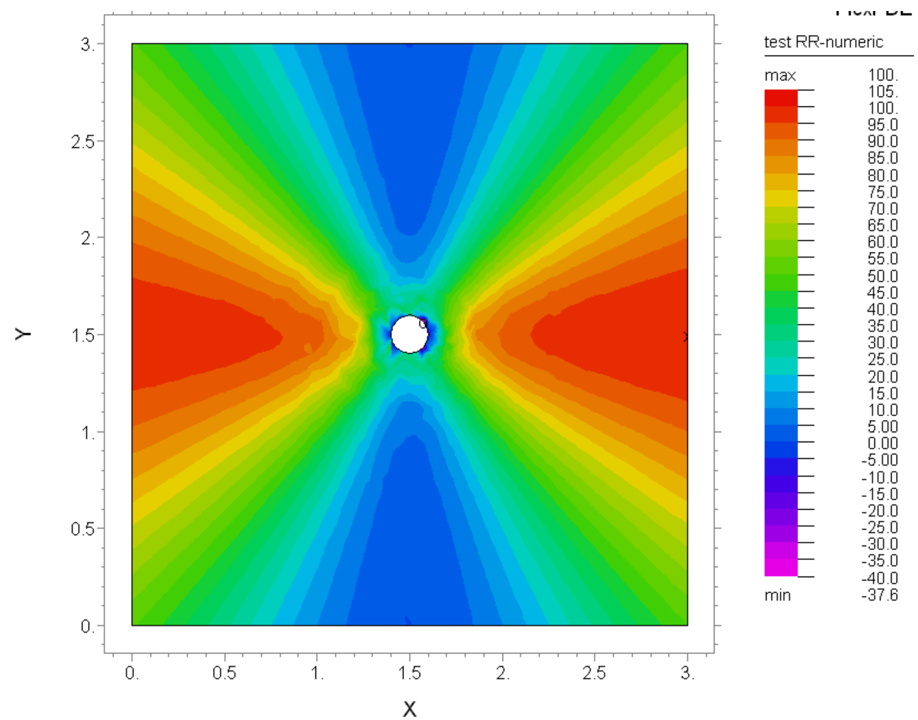
Example 2. The Kirsch problem

Tension of the Bar with a Hole



Analytical solution

σ_{RR}



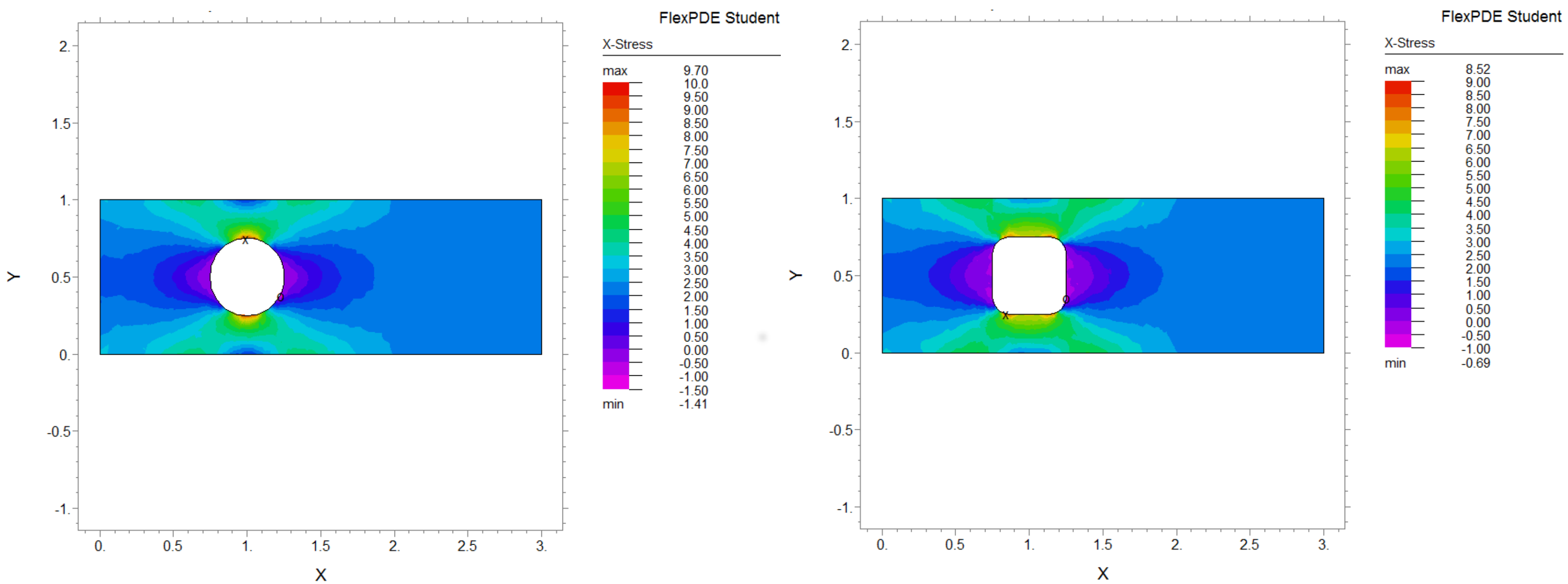
Numerical solution

σ_{RR}

Example 2. The Kirsch problem

Individual tasks: to analyze
the dependence of stress-strain state from

- geometrical parameters
- physical parameters
- boundary conditions

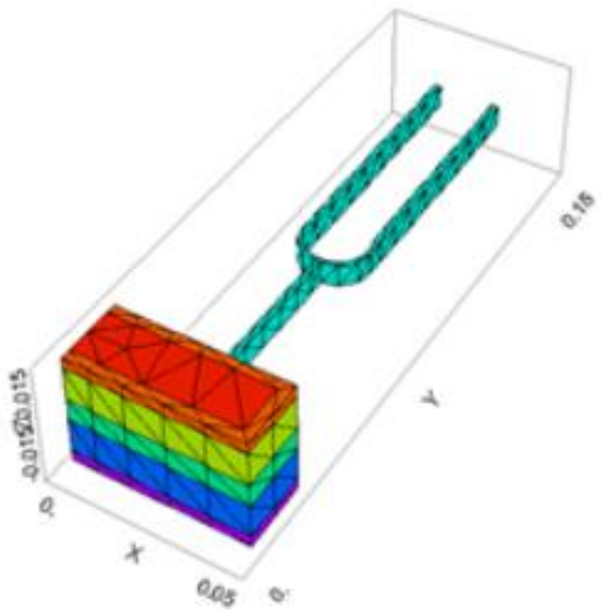


The dependence on the hole shape

Example 3. Frequency analysis

La 1st octave. Frequency - 440 Hz

Tuning fork with resonator box



3D model of the fork

Example 3. Frequency analysis

Equations of motion

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} = \rho \frac{\partial^2 \mathbf{u}}{\partial t^2}$$

Cauchy relations

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

Hooke's law

$$\sigma_{ij} = \lambda \theta + 2\mu \delta_{ij} \varepsilon_{ij}$$

Boundary conditions

- no forces on the side surface $\quad \mathbf{n} \cdot \boldsymbol{\sigma} = 0$
- no motion at the sealing $\quad \mathbf{u} = 0$

Stationary problem

$$\mathbf{u}(x, y, z, t) = \mathbf{u}(x, y, z) \cos(\omega t)$$

Example 3. Frequency analysis

```
COORDINATES
  cartesian3
 SELECT
    {numbers of frecuency}
    modes = 3
VARIABLES
  U1 U2 U3  { displacements }
DEFINITIONS
  nu=0.3
  E=200e9
  lambda=E/(1+nu)/(1-2*nu)
  mu=E/(2*(1+nu))
  ...
    { Cauchy relation }
    E11 = dx(U1)
    E12 =(dy(U1) + dx(U2))/2
    …
    { Hooke's law }
    S11=lambda*((1-nu)*E11+ nu*E22)
    S12=mu*E12
   ...
```

```
EQUATIONS
  U1: dx(S11) + dy(S12) + dz(S31) + Omega*rho*U = 0
  U2: dx(S12) + dy(S22) + dz(S32) + Omega*rho*V = 0
  U3: dx(S13) + dy(S23) + dz(S33) + Omega*rho*W = 0

EXTRUSION
z = 0, h
BOUNDARIES
 region 1
   start(0,0)
  { Boundary conditions }
   load(U1)=0 load(U2)=0 load(U3)=0 line to…
PLOTS
  grid(x+U1, y+U2, z+U3) as "Shape"...
summary
  report lambda
END
```

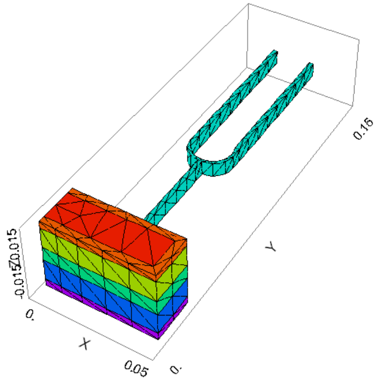
Example 3. Frequency analysis

Possible complicating

2D → 3D → 3D + Resonator

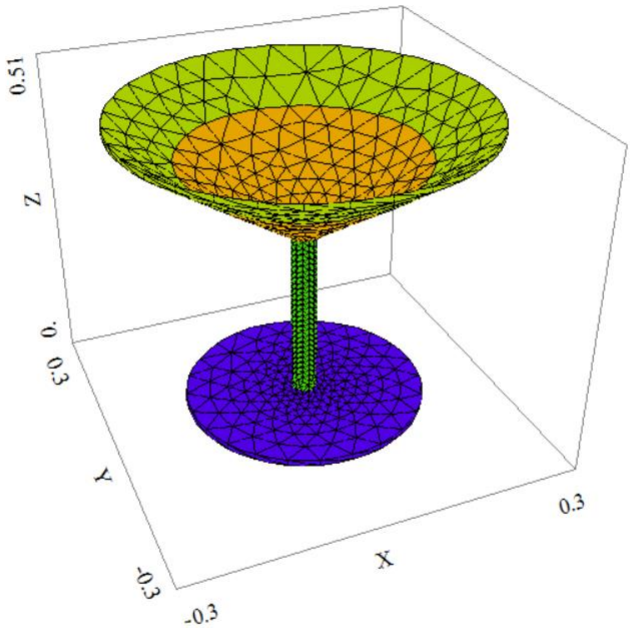
Individual tasks: to analyze
the dependence of frequency from

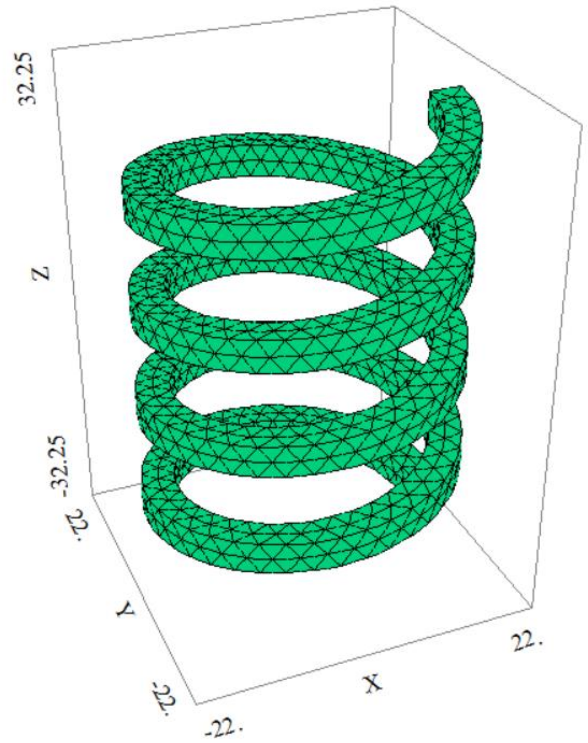
- geometrical parameters
- physical parameters
- boundary conditions



Additional tasks

Building of Geometry

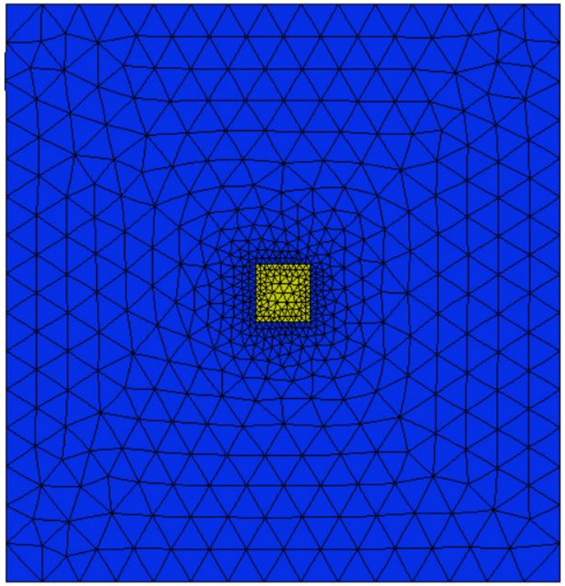




Export and import of Data

Additional tasks

Influence of grid parameters on the accuracy of the solution



- ✓ **CELL SIZE CONTROL**
- ✓ **MESH_DENSITY**
- ✓ **MESH_SPACING**
- ✓ **RESOLVE**
- ✓ **BDRY_DENSITY**
- ✓ **ERRLIM**

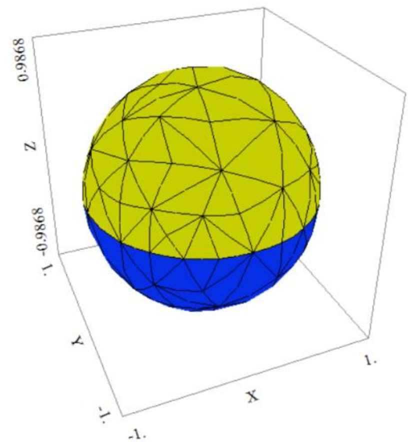
Analysis and further processing of the results

Additional tasks

Influence of grid parameters on the accuracy of the solution

Status

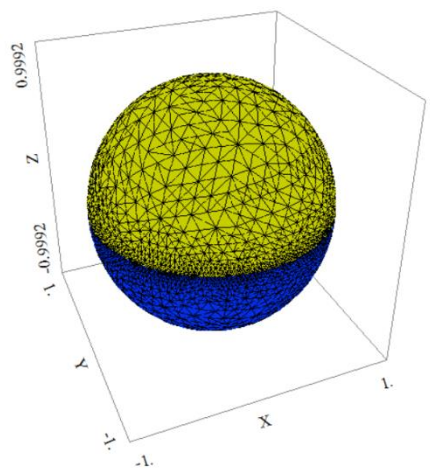
CPU time	0:08
Grid	1
Nodes	6243
Cells	4026
Unknowns	6243
Mem(K)	54349
RMS Error	1.228e-3
Max Error	4.647e-3
--DONE--	




```
select
   { error limit }
   errlim=1e-2
   { mesh size }
   ngrid=2
```

Status

CPU time	2:05
Grid	8
Nodes	270194
Cells	188346
Unknowns	270194
Mem(K)	475046
RMS Error	5.765e-5
Max Error	4.154e-4
--DONE--	




```
select
   { error limit }
   errlim=1e-4
   { mesh size }
   ngrid=4
```

Conclusion

So why we like FlexPDE package so much?

- **Student version is free**
- **The transparency of BVP solving allows to**
  - better absorb the course material
  - understand the essence of the problem
  - propose new ideas and methods of solution
  - attract additional math for solving complex problems

THANK YOU!

Olga Pustovalova, ogpustovalova@sfedu.ru

Mikhail Karyakin, karyakin@sfedu.ru

I.I.Vorovich Institute of Mathematics, Mechanics and Computer Science
Southern Federal University, Rostov-on-Don, Russia