Numerical solution of elliptic problems with non-classical interface conditions

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Introduction

Elliptic equations with classical boundary conditions (Dirichlet, Neumann, Robin and mixed types) have been studied for years.
In 1959 A. Venttsel introduced a new class of boundary conditions for elliptic equations. The boundary condition is a linear combination of the solution, its normal derivative and its second order tangential derivatives.
A simple example is the boundary problem:

$$\begin{aligned} -\Delta u(r) &= f(r), \quad r \in \Omega, \\ \alpha \frac{\partial^2 u}{\partial \tau^2}(r) - \beta u(r) - \frac{\partial u}{\partial n}(r) &= g(r), \quad r \in \partial\Omega. \end{aligned} \tag{1}$$

Ω - a bounded domain in $\mathbb{R}^2$ with a smooth boundary $\partial\Omega$; n - the outward normal to $\partial\Omega$; τ - the tangential direction to $\partial\Omega$.
The boundary condition in (1) is referred as "Venttsel boundary condition".

The specific nature of the considered problem:

- the boundary condition contains both the second order tangential derivative and the normal derivative.
- the boundary equation in (1) is not an autonomous equation on $\partial\Omega$.
- one cannot use directly the general theory of elliptic problems to get a-priori estimates.

In 1983 P. Korman mentioned:

- If $\alpha \leq 0$ and $\beta = 0$, then the problem is ill-posed in some sense.
- If $\alpha > 0$ and $\beta > 0$, then the problem is well-posed.

We assume here that $\alpha > 0$ and $\beta > 0$.

Elliptic problems with Venttsel type boundary conditions appear in numerous problems in:

- the water waves theory (Korman, P. (Nonlinear Analysis, Theory, Methods, & Applications, 7 1983), Shinbrot M. (J. Inst. Maths Applics, 25 (1980));
- engineering problems of oil wells (Cannon, J., Meyer, G., SIAM J. Appl. Math., 20 (1971));
- the heat transfer (Apushkinskaya, D., Nazarov, A., Applications of Mathematics, 45, (2000)).

Conditions of this type also appear as the interface condition between two sub-domains with different characteristics – "two phase problems":

- electrostatic process, connected with the functioning of the Atomic Force Microscope (AFM)

Unique solvability of problems with Venttsel condition is established:

- for the linear problem (1), in Hőlder spaces $C^{2,\epsilon}(\Omega)$ – by Luo and Trudinger (1991);
- for the quasilinear elliptic problems with the quasilinear Venttsel type boundary conditions in the Sobolev spaces $W_q^2(\Omega) \cap W_{q-1}^2(\partial\Omega)$ for $q > 2$ – by D. Apushkinskaya and A. Nazarov (1995);
- a survey of results on nonlinear elliptic and parabolic Venttsel problem can be found in Applications of Mathematics, 45(2000);
- for the two-phase quasilinear elliptic problems and parabolic Venttsel problems – by D. Apushkinskaya and A. Nazarov (2002).

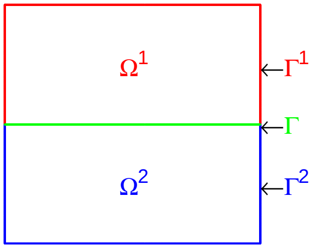
- numerical methods for one-phase Venttsel type elliptic problems: Kolkovska (2006)

In this talk:

- in the first part, we present a finite difference method for the numerical solution of the elliptic two-phase Venttsel type problem. We obtain error estimate of the method in the discrete energy norm V_h^1, which is optimal for solutions from V^2.
- in the second part, we apply the finite difference method for numerical simulation of some electrostatic processes connected with the functioning of the Atomic Force Microscope (AFM).

Preliminaries

Let Ω be the rectangle $(0,1) \times (-1,1)$ in R^2.
The interval $\Gamma = (0 < x < 1) \times (y = 0)$ separates the domain Ω into two parts, $\Omega^1 = (0,1) \times (0,1)$ and $\Omega^2 = (0,1) \times (-1,0)$.
Thus $\Omega = \Omega^1 \cup \Omega^2 \cup \Gamma$.
We introduce the notations $\Gamma^i = \partial\Omega^i \backslash \Gamma$, $i = 1,2$, for the parts of sub-domains' boundaries.



As usually, by $H^k(\Omega)$ and $H^k(\Gamma)$ we denote the Sobolev spaces on Ω or on Γ. For the two sub-domains of Ω we introduce the spaces

$$H^k_{\Gamma^i}(\Omega^i) = \left\{ u \in H^k(\Omega^i) : u\,|_{\Gamma^{(i)}} = 0 \right\},\; i = 1, 2,\; k = 1, 2, 3.$$

For functions on Ω, whose restrictions on Ω^i belong to the above spaces, we set

$$V^k = \left\{ u = (u^{(1)}, u^{(2)}) : u^{(i)} \in H^k{}_{\Gamma^i}(\Omega^i), i = 1, 2, \right.$$
$$\left. u^{(1)}\Big|_\Gamma = u^{(2)}\Big|_\Gamma \in H^k(\Gamma) \right\}, \quad k = 1, 2, 3.$$

The spaces V^k, $k = 1, 2, 3$, are equipped with the norm

$$\|u\|_{V^k} = \left| u^{(1)} \right|_{H^k(\Omega^1)} + \left| u^{(2)} \right|_{H^k(\Omega^2)} + \|u\|_{H^k(\Gamma)} .$$

Formulation of the two-phase problem

We consider the elliptic problem with discontinuous coefficients

$$-\frac{\partial}{\partial x}a^{(i)}\frac{\partial u^{(i)}}{\partial x}(r)-\frac{\partial}{\partial y}b^{(i)}\frac{\partial u^{(i)}}{\partial y}(r)=f^{(i)}(r),\ r\in\Omega^{i},\ i=1,2 \quad (2)$$

subjected to the boundary conditions

$$u^{(i)}(r)=0,\ r\in\Gamma^{i},\quad i=1,2, \quad (3)$$

and the interface condition of Venttsel type on Γ

$$u^{(1)}(r)=u^{(2)}(r)=u(r),\quad r\in\Gamma, \quad (4)$$

$$\alpha\frac{\partial^2 u}{\partial x^2}(r)-\beta u(r)-b^{(1)}\frac{\partial u^{(1)}}{\partial y}(r)+b^{(2)}\frac{\partial u^{(2)}}{\partial y}(r)=g(r),\quad r\in\Gamma. \quad (5)$$

Here α, β and $a^{(i)}, b^{(i)}$, $i=1,2$, are positive constants.

The weak form of boundary problem (2)–(5) is:
Find a function $u \in V^1$ such that

$$a(u,v) = \sum_{i=1,2} \int_{\Omega^i} f^{(i)}(x,y) v^{(i)}(x,y)\,dxdy + \int_{\Gamma} g(x)v(x)\,dx, \quad \forall v \in V^1,$$

where the bilinear form $a(u,v)$ is

$$a(u,v) = \sum_{i=1,2} \int_{\Omega^i} \left[a^{(i)} \frac{\partial u^{(i)}(x,y)}{\partial x} \frac{\partial v^{(i)}(x,y)}{\partial x} + b^{(i)} \frac{\partial u^{(i)}(x,y)}{\partial y} \frac{\partial v^{(i)}(x,y)}{\partial y} \right] dxdy$$

$$+ \int_{\Gamma} \left(\alpha \frac{\partial u(x,0)}{\partial x} \frac{\partial v(x,0)}{\partial x} + \beta u(x,0)v(x,0) \right) dx, \quad u,v \in V^1.$$

There exists an unique generalized solution to (2)–(5).

Lemma

Let $f^{(i)} \in L_2(\Omega^i), i = 1,2,$ and $g \in H^{\frac{1}{2}}(\Gamma)$. Then the boundary problem (2)–(5) has a unique strong solution $u \in V^2$.

Formulation of the numerical method

We introduce a uniform mesh $\overline{\omega}_h$ in $\overline{\Omega}$ with mesh sizes $h = (h_1, h_2)$, $h_i = N_i^{-1}, N_i \in N, i = 1, 2$, which is aligned with the interface Γ.
We set $\omega_h^{(i)} = \overline{\omega}_h \cap \Omega^i$, $\gamma_h^{(i)} = \overline{\omega}_h \bigcap \Gamma^i$, $i = 1, 2$, $\gamma_h = \overline{\omega}_h \bigcap \Gamma$.
Thus $\overline{\omega}_h = \omega_h^{(1)} \cup \omega_h^{(2)} \cup \gamma_h^{(1)} \cup \gamma_h^{(2)} \cup \gamma_h$.
We denote by $\mathring{\mathrm{H}}_h$ the set of discrete functions, defined on $\overline{\omega}_h$, which vanish on $\gamma_h^{(1)} \cup \gamma_h^{(2)}$, with the scalar product

$$(u, v)_h = \sum_{r \in \omega_h^{(1)} \cup \omega_h^{(2)}} h_1 h_2 u(r) v(r) + \sum_{r \in \gamma_h} h_1 h_2 u(r) v(r).$$

Let V_h^1 be the discrete analog to the space V^1 with the norm

$$\|z\|^2_{V_h^1} = [z_x, z_x)_h + [z_y, z_y)_h + \sum_{r \in \gamma_h \bigcup (0,0)} h_1 (z^2 + z_x^2)(r).$$

We approximate the problem (2)-(5) with the finite difference scheme

$$\begin{aligned} A_h v \equiv A_1 v(r) + A_2 v(r) &= \varphi(r), \quad r \in \omega_h^{(1)} \cup \omega_h^{(2)} \cup \gamma_h, \\ v(r) &= 0, \qquad\quad r \in \gamma_h^{(1)} \cup \gamma_h^{(2)}, \end{aligned} \tag{6}$$

where

$$A_1 v(r) = -\begin{cases} (a^{(1)} v_{\bar{y}})_y(r), & r \in \omega_h^{(1)}, \\ (a^{(2)} v_{\bar{y}})_y(r), & r \in \omega_h^{(2)}, \\ \left(\frac{a^{(1)}+a^{(2)}}{2} + \frac{\alpha}{h_2}\right) v_{x\bar{x}}(r), & r \in \gamma_h, \end{cases}$$

$$A_2 v(r) = -\begin{cases} (b^{(1)} v_{\bar{y}})_y(r), & r \in \omega_h^{(1)}, \\ (b^{(2)} v_{\bar{y}})_y(r), & r \in \omega_h^{(2)}, \\ \frac{1}{h_2}(b^{(1)} v_y - b^{(2)} v_{\bar{y}}) - \frac{\beta}{h_2} v(r), & r \in \gamma_h, \end{cases}$$

$$\varphi(r) = \begin{cases} T_1 T_2 f^{(1)}(r), & r \in \omega_h^{(1)}, \\ T_1 T_2 f^{(2)}(r), & r \in \omega_h^{(2)}, \\ T_1 T_2^+ f^{(1)}(r) + T_1 T_2^- f^{(2)}(r) - \frac{1}{h_2} T_1 g(r), & r \in \gamma_h. \end{cases}$$

The averaging operators T_1, T_2, T_2^+, T_2^- are defined for functions v from L_1. At $r = (x, y)$ they are:

$$T_1 v(r) = \int_{-1}^{1} (1-|s|) v(x+sh_1, y) ds, \; T_2 v(r) = \int_{-1}^{1} (1-|s|) v(x, y+sh_2) ds,$$

$$T_2^+ v(r) = \int_{0}^{1} (1-s) v(x, y+sh_2) ds, \; T_2^- v(r) = \int_{-1}^{0} (1+s) v(x, y+sh_2) ds.$$

The finite difference scheme (6) is obtained by discretization of the balance equation over control volumes . Thus, the resulting discrete operator preserves the important properties of the continuous one.

Lemma

For all $u, v \in \mathring{H}_h$ the discrete operator A_h satisfies the identity

$$\begin{aligned}(A_h u, v)_h &= a^{(1)}[u_x, v_x)_{h,(j>0)} + a^{(2)}[u_x, v_x)_{h,(j<0)} \\ &+ b^{(1)}[u_y, v_y)_{h,(j\geq 0)} + b^{(1)}[u_y, v_y)_{h,(j<0)} \\ &+ \beta \sum_{r\in\gamma_h} h_1 u(r) v(r) \\ &+ \left\{\alpha + \frac{a^{(1)} + a^{(2)}}{2} h_2\right\} \sum_{r\in\gamma_h \bigcup (0,0)} h_1 u_x(r) v_x(r).\end{aligned}$$

A_h is a self-adjoint positive definite operator on $\mathring{H}_h$.

The proof follows by partial summation and uses the assumptions $\alpha > 0$ and $\beta > 0$.

A consequence of the Lemma: there exists a unique solution to the difference scheme (6).

Rate of convergence of the finite difference scheme

Theorem

Let $u \in V^k$, $k = 2, 3$ be the solution of (2)–(5) and let v be the solution of the finite difference method (6). There exists a positive constant C (independent on u, v and h) such that

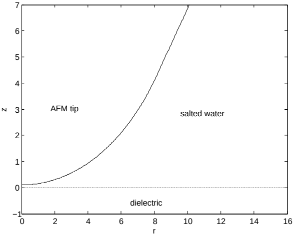
$$\|v - u\|_{V_h^1} \leq C|h|^1 \|u\|_{V^2}, \quad \|v - u\|_{V_h^1} \leq C|h|^{1.5} \|u\|_{V^3}.$$

- in the case $k = 2$ the rate of convergence is consistent with the smoothness of the exact solution;.
- in the case $k = 3$ there is a loss of the order of convergence of $O(h^{-0.5})$.
- the rate of convergence is the same as for the elliptic problem with Robin boundary condition.

The proof is based on a-priori estimates, analysis of the error of approximation and the Bramble-Hilbert lemma.

Mathematical model

We consider an Atomic Force Microscope (AFM) probing a dielectric. Then three sub-domains appear – the AFM tip, water and dielectric. We suppose that the AFM tip is a cone with a spherical end, and the problem is axisymmetric.



In each sub-domain the equation for the potential $\varphi(r, z)$ (in cylindrical coordinates (r, z)) is

$$\varepsilon \nabla^2 \varphi = \varepsilon \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \varphi}{\partial r} + \varepsilon \frac{\partial^2 \varphi}{\partial^2 z} = k^2 \varphi,$$

where k is the reciprocal Debye length of the corresponding medium.

The surface dielectric permittivities modify the conditions of the Gauss law. Thus at the surface AFM tip-water (defined by $z = z_s(r)$) the corresponding interface condition becomes

$$D_N^+ - D_N^- + \varepsilon^s \boldsymbol{\nabla}^{\mathbf{s}} \cdot \mathbf{D}^{\mathbf{s}} = \rho^s,$$

where

$$D_N^\pm = -\varepsilon^\pm \mathbf{n} \cdot \boldsymbol{\nabla} \varphi^\pm = -\varepsilon^\pm \frac{1}{\sqrt{1 + {z_s'}^2}} \left(\frac{\partial \varphi^\pm}{\partial z} - z_s' \frac{\partial \varphi^\pm}{\partial r} \right),$$

$$\boldsymbol{\nabla}^{\mathbf{s}} \cdot \mathbf{D}^{\mathbf{s}} = \frac{\partial^2 \varphi^s}{\partial \tau^2} = -\frac{1}{r\sqrt{1 + {z_s'}^2}} \frac{d}{dr} \left(\frac{r}{\sqrt{1 + {z_s'}^2}} \frac{d\varphi^s}{dr} \right).$$

Here $\varphi^s(r) = \varphi(r, z_s(r))$ is the restriction of the potential over the surface.

On the water-dielectric surface $z_s' = 0$ and the corresponding interface condition becomes

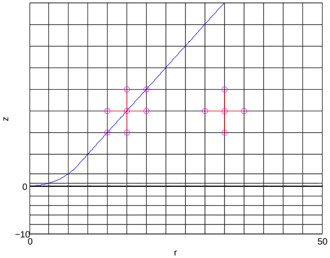
$$-\varepsilon^{+}\frac{\partial\varphi^{+}}{\partial z} + \varepsilon^{-}\frac{\partial\varphi^{-}}{\partial z} - \varepsilon^{s}\frac{1}{r}\frac{d}{dr}r\frac{d\varphi^{s}}{dr} = \rho^{s};$$

The interface conditions on both surfaces (AFM tip-water) and (water-dielectric) are of Venttsel's type.

We equip the problem with boundary conditions on the top, bottom and the right boundaries.

Numerical method

We use a nonuniform rectangular grid so that the interface coincides either with lines of the grid or with diagonals of the rectangles. A 5-point discrete Laplacian scheme is used for approximation at the interior mesh points.

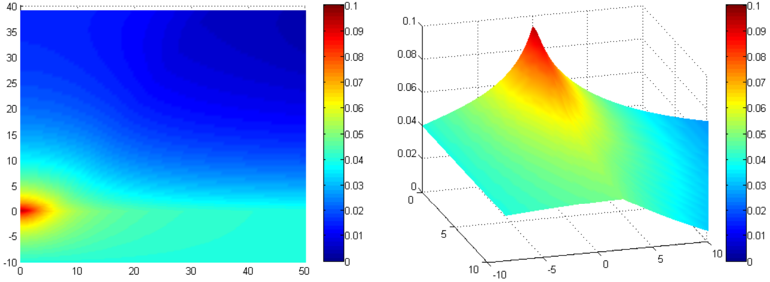


For the approximation of the interface condition we use the balance equation and two additional neighbor mesh points.
It turns out that at the mesh points on the water-dielectric surface the resulting scheme coincides with the FD scheme considered in the first part.
The linear system obtained after discretization is solved using ILU preconditioned BiCGStab method.

Numerical results

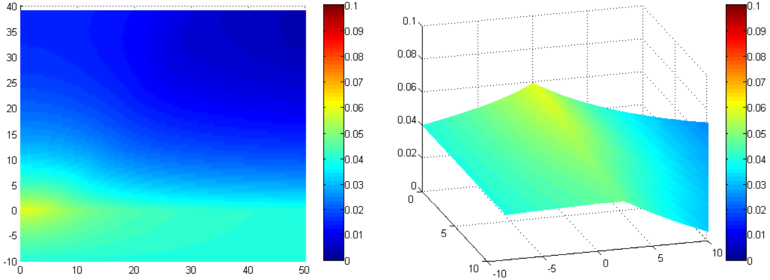
We consider the mathematical model with the following physical parameters:
the end of the tip – sphere with $R = 10$ nm,
the distance between the tip and the dielectric – $d = 0.1$ nm
$k = 0$, $\varepsilon = 2\,\text{nm}$ in the AFM tip sub-domain
$k = 0.07\,\text{nm}^{-1}$, $\varepsilon = 80\,\text{nm}$ in the water
$k = 0$, $\varepsilon = 2\,\text{nm}$ in the dielectric
$\rho = 0$ on the tip-water surface
$\rho = 0.224\,\text{V/nm}$ on the water-dielectric surface;
sequence of embedded grids $\ell = 0, 1, 2, \ldots, 6$
the maximum of the potential is at $(r, z) = (0, 0)$.

The solution for $\varepsilon^s = 0$ on both surfaces



The second order tangential derivative in the interface condition (surface dielectric permittivities) is neglected.

The solution for $\varepsilon^s = 100$ on both surfaces



The second order tangential derivative in the interface conditions (surface dielectric permittivities) are included in the model.
The surface dielectric permittivities influence essentially the potential.

Numerical tests

- We check numerically the accuracy of the method.
  The numerical results shown on next tables confirm the theoretical order of convergence of the method.
- We have studied the influence of some physical parameters on the potential field:
  - the form of the AFM tip (the radius of the spherical end)
  - the distance between the the AFM tip and the dielectric

  The numerical results show that surface dielectric permittivities influence essentially the potential; this influence is stronger when the distance between the AFM tip and the dielectric surface is smaller.

Examples 1-2

		$\varepsilon^s = 0$			$\varepsilon^s = 100\,\mathrm{nm}$		
ℓ	#points	$\varphi(0,0)$	$\lvert\varphi_{\ell-1} - \varphi_\ell\rvert$	κ	$\varphi(0,0)$	$\lvert\varphi_{\ell-1} - \varphi_\ell\rvert$	κ
0	336	1.3580e-1			6.4617e-2		
1	1271	1.0492e-1	0.3088e-1		6.1355e-2	0.3262e-2	
2	4941	9.6612e-2	0.8308e-2	1.89	6.0014e-2	0.1341e-2	1.28
3	19481	9.3397e-2	0.3215e-2	1.37	5.9337e-2	0.0677e-2	0.99
4	77361	9.1870e-2	0.1527e-2	1.07	5.9000e-2	0.0337e-2	1.01
5	308321	9.1118e-2	0.0752e-2	1.02	5.8834e-2	0.0166e-2	1.02

where

$$\kappa = \log_2 \frac{\lvert\varphi_{\ell-1} - \varphi_{\ell-2}\rvert}{\lvert\varphi_\ell - \varphi_{\ell-1}\rvert}.$$

$$\varepsilon^s = 0$$

ℓ	#points	$\varphi(3.33,0)$	$e_\ell(3.33,0)$	κ	E_ℓ	κ	E'_ℓ	κ
0	336	6.7360e-2						
1	1271	7.0458e-2	3.10e-3		1.35e-2		4.01e-3	
2	4961	7.1419e-2	9.61e-4	1.69	4.19e-3	1.69	2.35e-3	0.77
3	19481	7.1671e-2	2.52e-4	1.93	1.10e-3	1.92	1.15e-3	1.04
4	77361	7.1735e-2	6.35e-5	1.99	2.81e-3	1.97	5.87e-3	0.97
5	308321	7.1751e-2	1.60e-5	1.99	7.10e-5	1.98	2.99e-4	0.97
6	1231041	7.1755e-2	4.00e-6	2.00	1.78e-5	2.00	1.51e-4	0.99

$$e_\ell(r,z) = |\varphi_{\ell-1}(r,z) - \varphi_\ell(r,z)|,$$

$$(E_\ell)^2 = \int_0^{10} r(\varphi_{\ell-1}(r,0) - \varphi_\ell(r,0))^2 \, dr,$$

$$(E'_\ell)^2 = \int_0^{10} r\left(\frac{\partial\varphi_{\ell-1}}{\partial r}(r,0) - \frac{\partial\varphi_\ell}{\partial r}(r,0)\right)^2 \, dr.$$

$$\varepsilon^s = 100$$

l	#points	$\varphi(3.33, 0)$	$e_\ell(3.33, 0)$	κ	$E_\ell(0)$	κ	$E'_\ell(0)$	κ
0	336	5.5444e-2						
1	1271	5.6205e-2	7.61e-4		4.70e-3		6.10e-4	
2	4961	5.6416e-2	2.11e-4	1.85	1.31e-3	1.84	3.26e-4	0.91
3	19481	5.6469e-2	5.28e-5	2.00	3.32e-4	1.98	1.69e-4	0.95
4	77361	5.6482e-2	1.30e-5	2.02	8.20e-5	2.02	8.55e-5	0.98
5	308321	5.6485e-2	3.29e-6	1.98	2.07e-5	1.99	4.29e-5	0.99
6	1231041	5.6486e-2	8.20e-7	2.00	5.16e-6	2.00	2.15e-5	1.00

$$e_\ell(r, z) = |\varphi_{\ell-1}(r, z) - \varphi_\ell(r, z)|,$$

$$(E_\ell)^2 = \int_0^{10} r(\varphi_{\ell-1}(r, 0) - \varphi_\ell(r, 0))^2 \, \mathrm{d}r,$$

$$(E'_\ell)^2 = \int_0^{10} r \left(\frac{\partial \varphi_{\ell-1}}{\partial r}(r, 0) - \frac{\partial \varphi_\ell}{\partial r}(r, 0) \right)^2 \, \mathrm{d}r.$$

Example 3

$R = 100$ nm, the computational domain is twice larger in r direction.

		$\varepsilon^s = 100\,\text{nm}$		
ℓ	#points	$\varphi(0,0)$	$\lvert\varphi_{\ell-1} - \varphi_\ell\rvert$	κ
0	336	1.9740e-1		
1	1271	1.8536e-1	0.1204e-1	
2	4961	1.7936e-1	0.0600e-1	1.00
3	19481	1.7637e-1	0.0299e-1	1.00
4	77361	1.7488e-1	0.0149e-1	1.00
5	308321	1.7413e-1	0.0075e-1	0.99

Example 4

The distance between the AFM tip and the dielectric surface is $d = 1$ nm.

		$\varepsilon^s = 0$			$\varepsilon^s = 100\,\text{nm}$		
ℓ	#points	$\varphi(0,0)$	$\lvert\varphi_{\ell-1} - \varphi_\ell\rvert$	κ	$\varphi(0,0)$	$\lvert\varphi_{\ell-1} - \varphi_\ell\rvert$	k
0	336	7.7059e-2			5.9538e-2		
1	1271	7.0744e-2	0.6315e-2		5.6734e-2	0.2804e-2	
2	4961	6.8368e-2	0.2376e-2	1.41	5.5597e-2	0.1137e-2	1.30
3	19481	6.7226e-2	0.1142e-2	1.06	5.5024e-2	0.0573e-2	0.99
4	77361	6.6661e-2	0.0565e-2	1.02	5.4737e-2	0.0287e-2	1.00
5	308321	6.6381e-2	0.0280e-2	1.01	5.4594e-2	0.0143e-2	1.01

Remarks and conclusions

1. A finite difference method for solving elliptic problems with non-classical interface conditions in rectangular domains is proposed.
The obtained error estimate of the method in the discrete energy norm V_h^1 is consistent with the smoothness of solutions from V^2.
2. In the present talk we restrict ourselves to problem with partially constant coefficients (to demonstrate the properties of the method). In a similar way we can handle the general case of elliptic problems with variable coefficients.
Future work includes:

- Testing other shapes for the end of the AFM tip;
- Comparison with experiments;
- Solving real 3D problems (the tip is usually a pyramid).

THANK YOU !