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BENCHMARK SOLUTIONS FOR NANOFLOWS

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Essential viscosity variation creates additional difficulties for numerical investigation of flows through nanotubes and nanochannels. Benchmark solutions of the Stokes and continuity equations with variable viscosity are suggested. This is useful for testing of numerical algorithms applied to this problem.

Keywords: nanotube, Stokes flow, benchmark solution.

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1. Introduction

Flows through nanotubes and other nanostructures have many interesting peculiarities. One of them is the viscosity variation (see, e.g., [1], [2], [3]). Flows in nano-channels are influenced by local heterogeneity of molecular structure of the liquid if its size is compared with the channel width. A hypothesis about the existence of locally-ordered structures in liquid was put forward in [4]. Investigations of fluid flows in nano-sized domains show that it is strongly influenced by local ordering of nano-sized scale. Experiments [5], [6] show that the effective viscosity of water in nanochannel with hydrophilic walls is essentially greater than the corresponding macroscopic value. Experimental and theoretical investigations of water state in carbon nanotube [7], [8] show that there is an ice-like envelope with liquid water inside in the nanotube. Increasing of effective fluid viscosity via channel diameter was marked in [9] for channels of a few micrometers diameters. Thus, experiments confirm high viscosity variations for the flow in a nanotube, which creates computational problems. Namely, the convergence of the numerical algorithms in the case of strongly varying viscosity is not good, and, moreover, is not guaranteed ([10], [11]). Correspondingly, one need an instrument to choose an appropriate numerical scheme. One can make a choice by using of benchmark solutions (see, e.g., [12], [13], [14])

In present work, we suggest methods for algorithm checking. The scheme of the algorithm testing is as follows. Consider a rectangular domain. Calculate the values of the benchmark solutions at the rectangle's boundary. Take these values as the boundary conditions. Due to the uniqueness theorem the solution of the boundary problem should coincide with our benchmark solution. So, we obtain a solution of the specific boundary problem. Note that we derived the solution analytically. Next, we solve the same boundary problem by a numerical algorithm, then we compare results and estimate the quality of the numerical algorithm.

We have found exact analytical solutions of the Stokes and continuity equations in the two-dimensional case for linearly varying viscosity. These solutions are convenient to use as benchmarks for numerical algorithm testing. The efficiency of the approach was demonstrated on a numerical algorithm for calculations of the Stokes flow with varying viscosity.

2. Formulation of Stokes and continuity equations with variable viscosity

Consider the plane flow. 2D Stokes equations for the case of varying viscosity has the form:

$$2\eta\frac{\partial^2 v_x}{\partial x^2}+2\frac{\partial\eta}{\partial x}\frac{\partial v_x}{\partial x}+\eta\frac{\partial^2 v_x}{\partial y^2}+\eta\frac{\partial^2 v_y}{\partial y\partial x}+\frac{\partial\eta}{\partial y}\frac{\partial v_x}{\partial y}+ \\ \frac{\partial\eta}{\partial y}\frac{\partial v_y}{\partial x}-\frac{\partial P}{\partial x}=-\rho G_x, \tag{1}$$

$$\eta\frac{\partial^2 v_y}{\partial x^2}+\eta\frac{\partial^2 v_x}{\partial y\partial x}+\frac{\partial\eta}{\partial x}\frac{\partial v_x}{\partial y}+\frac{\partial\eta}{\partial x}\frac{\partial v_y}{\partial x}+2\frac{\partial\eta}{\partial y}\frac{\partial v_y}{\partial y}+ \\ 2\eta\frac{\partial^2 v_y}{\partial y^2}-\frac{\partial P}{\partial y}=-\rho G_y, \tag{2}$$

$$\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}=0. \tag{3}$$

Here (v_x, v_y) is the flow velocity, $\eta=\eta(x,y)$ is the viscosity, P is the pressure, ρ is the density, (G_x, G_y) is the gravitational force. Note that (3) is the continuity equation.

Let us change the variables v_x, v_y, P in such a way that:

$$\frac{\partial v_x}{\partial x}=\frac{1}{\eta}\frac{\partial u_x}{\partial x},\quad \frac{\partial v_x}{\partial y}=\frac{1}{\eta}\frac{\partial u_x}{\partial y}, \tag{4}$$

$$\frac{\partial v_y}{\partial x}=\frac{1}{\eta}\frac{\partial u_y}{\partial x},\quad \frac{\partial v_y}{\partial y}=\frac{1}{\eta}\frac{\partial u_y}{\partial y}. \tag{5}$$

$$\frac{1}{\eta}\frac{\partial P}{\partial x}=\frac{\partial \tilde{P}}{\partial x},\quad \frac{1}{\eta}\frac{\partial P}{\partial y}=\frac{\partial \tilde{P}}{\partial y}. \tag{6}$$

The correctness conditions for such replacement are as follows:

$$\frac{\partial}{\partial y}(\frac{1}{\eta}\frac{\partial u_x}{\partial x})=\frac{\partial}{\partial x}(\frac{1}{\eta}\frac{\partial u_x}{\partial y}),\quad \frac{\partial}{\partial y}(\frac{1}{\eta}\frac{\partial u_y}{\partial x})=\frac{\partial}{\partial x}(\frac{1}{\eta}\frac{\partial u_y}{\partial y}),$$

$$\frac{\partial}{\partial y}(\eta\frac{\partial \tilde{P}}{\partial x})=\frac{\partial}{\partial x}(\eta\frac{\partial \tilde{P}}{\partial y}).$$

These conditions lead to the following correlations:

$$\frac{\partial\eta}{\partial y}\frac{\partial u_x}{\partial x}=\frac{\partial\eta}{\partial x}\frac{\partial u_x}{\partial y},\quad \frac{\partial\eta}{\partial y}\frac{\partial u_y}{\partial x}=\frac{\partial\eta}{\partial x}\frac{\partial u_y}{\partial y},$$

$$\frac{\partial\eta}{\partial y}\frac{\partial \tilde{P}}{\partial x}=\frac{\partial\eta}{\partial x}\frac{\partial \tilde{P}}{\partial y}.$$

All conditions give one the same characteristic equation:

$$\frac{\partial\eta}{\partial x}dx+\frac{\partial\eta}{\partial y}dy=0.$$

Evidently, $\eta(x,y)=C$ is an integral of the equation. Hence, the solutions of our equations, which predetermine the correctness of replacement suggested above, are

$$u_x=\Phi(\eta),\quad u_y=\Psi(\eta),\quad \tilde{P}=\tilde{P}(\eta).$$

After replacement, the Stokes equations (1), (2) and the continuity condition (3) transform to the following form:

$$2\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_y}{\partial y \partial x} - \eta\frac{\partial \tilde{P}}{\partial x} = -\rho G_x, \tag{7}$$

$$\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_x}{\partial y \partial x} + 2\frac{\partial^2 u_y}{\partial y^2} - \eta\frac{\partial \tilde{P}}{\partial y} = -\rho G_y, \tag{8}$$

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0. \tag{9}$$

Inserting the expressions for u_x, u_y into (7), (8), (9), one obtains the following equations:

$$\begin{aligned} &2\Phi'\frac{\partial^2 \eta}{\partial^2 x} + 2\Phi''\left(\frac{\partial \eta}{\partial x}\right)^2 + \Phi'\frac{\partial^2 \eta}{\partial^2 y} + \Phi''\left(\frac{\partial \eta}{\partial y}\right)^2 + \\ &\Psi'\frac{\partial^2 \eta}{\partial y \partial x} + \Psi''\frac{\partial \eta}{\partial y}\frac{\partial \eta}{\partial x} - \eta\tilde{P}'\frac{\partial \eta}{\partial x} = -\rho G_x, \end{aligned} \tag{10}$$

$$\begin{aligned} &2\Psi'\frac{\partial^2 \eta}{\partial^2 y} + 2\Psi''\left(\frac{\partial \eta}{\partial y}\right)^2 + \Psi'\frac{\partial^2 \eta}{\partial^2 x} + \Psi''\left(\frac{\partial \eta}{\partial x}\right)^2 + \\ &\Phi'\frac{\partial^2 \eta}{\partial y \partial x} + \Phi''\frac{\partial \eta}{\partial y}\frac{\partial \eta}{\partial x} - \eta\tilde{P}'\frac{\partial \eta}{\partial y} = -\rho G_y, \end{aligned} \tag{11}$$

$$\Phi'\frac{\partial \eta}{\partial x} + \Psi'\frac{\partial \eta}{\partial y} = 0. \tag{12}$$

3. Exponentially varying viscosity

Let us construct the second benchmark solution. Next, we assume that the viscosity is the exponential function of the Cartesian coordinates:

$$\eta = c\exp{(ax + by)}. \tag{13}$$

General consideration up to (10), (11), (12) is the same as earlier. By inserting (13) into (10), (11), (12) and taking into account that:

$$\frac{\partial \eta}{\partial x} = a\eta, \quad \frac{\partial \eta}{\partial y} = b\eta,$$

one obtains the following system of equations:

$$\begin{gathered} (2a^2 + b^2)(\Phi"\eta^2 + \Phi'\eta) + ab(\Psi"\eta^2 + \Psi'\eta) - a\tilde{P}'\eta^2 = -\rho G_x, \\ ab(\Phi"\eta^2 + \Phi'\eta) + (a^2 + 2b^2)(\Psi"\eta^2 + \Psi'\eta) - b\tilde{P}'\eta^2 = -\rho G_y, \\ a\Phi' + b\Psi' = 0. \end{gathered}$$

Using the last relation, we exclude Ψ from the first two equations:

$$\begin{gathered} (a^2 + b^2)(\Phi"\eta^2 + \Phi'\eta) - a\tilde{P}'\eta^2 = -\rho G_x, \\ -\frac{a^3 + ab^2}{b}(\Phi"\eta^2 + \Phi'\eta) - b\tilde{P}'\eta^2 = -\rho G_y, \\ \Psi' = -\frac{a}{b}\Phi'. \end{gathered} \tag{14}$$

One can see that we obtain a linear algebraic system with respect to $(\Phi"\eta^2 + \Phi'\eta)$ and $\tilde{P}'$. The solution is as follows:

$$\tilde{P}' = \frac{f_1(\eta)}{\eta^2}, \tag{15}$$

$$\Phi"\eta^2 + \Phi'\eta = bf(\eta). \tag{16}$$

Remark. It is interesting that these formulas contain the same functions $f(\eta)$, $f_1(\eta)$.

Equation (16) is a well-known Euler ordinary differential equation. One can get its solution for arbitrary function f:

$$u_x = \Phi(\eta) = b\int_1^\eta \log(\frac{\eta}{\eta_1})\frac{f(\eta_1)}{\eta_1}d\eta_1 + bc_1\log\eta + c_2. \tag{17}$$

Taking into account relation (14), one obtains u_y:

$$u_y = \Psi(\eta) = -a\int_1^\eta \log(\frac{\eta}{\eta_1})\frac{f(\eta_1)}{\eta_1})d\eta_1 - ac_1\log\eta + c_3. \tag{18}$$

Taking into account (4), (5), one obtains v_x, v_y:

$$v_x = b\int_1^\eta \frac{d\eta_1}{\eta_1^2}\int_1^{\eta_1} d\eta_2 \quad \frac{f(\eta_2)}{\eta_2} - bc_1\frac{1}{\eta} + bc_1 + c_2 =$$

$$b\int_1^\eta d\eta_2 \quad \frac{f(\eta_2)}{\eta_2}\int_{\eta_2}^\eta \frac{d\eta_1}{\eta_1^2} - bc_1\frac{1}{\eta} + bc_1 + c_2.$$

Hence, we get the expression for v_x and analogously, for v_y:

$$v_x = b\int_1^\eta d\eta_2 \quad \frac{f(\eta_2)}{\eta_2}\frac{\eta - \eta_2}{\eta\eta_2} - bc_1\frac{1}{\eta} + bc_1 + c_2, \tag{19}$$

$$v_y = -a\int_1^\eta d\eta_2 \quad \frac{f(\eta_2)}{\eta_2}\frac{\eta - \eta_2}{\eta\eta_2} + ac_1\frac{1}{\eta} + c_3. \tag{20}$$

As for the pressure, we obtain it from (15) by taking into account (6):

$$\tilde{P} = \int_1^\eta d\eta_1\frac{f_1(\eta_1)}{\eta_1^2} + c_4.$$

Hence,

$$P = \int_1^\eta d\eta_1\frac{f_1(\eta_1)}{\eta_1} + c_4. \tag{21}$$

For a simple particular case (constant gravitational term), when $f(\eta) = A = const$, $f_1(\eta) = A_1 = const$ one has:

$$v_x = -\frac{b(A + c_1)}{\eta} - \frac{bA\log\eta}{\eta} + \tilde{c}_2,$$

$$v_y = \frac{a(A + c_1)}{\eta} + \frac{aA\log\eta}{\eta} + \tilde{c}_3,$$

$$P = A_1\log\eta + c_4 - b_1,$$

A more complicated case is when the density is a linear function of the viscosity, $\rho = \beta_1\eta + \beta_2$, i.e.

$$f(\eta) = a_1\eta + a_2, \quad f_1(\eta) = b_1\eta + b_2,$$

where constants a_1, a_2, b_1, b_2 are the same as in the previous section. It is simple to evaluate integrals in (19), (20), (21). In such a way, one obtains:

$$v_x = ba_1\log\eta + \frac{b(a_1 - a_2 - c_1)}{\eta} - ba_2\frac{\log\eta}{\eta} + \tilde{c}_2,$$

$$v_y = -aa_1 \log \eta - \frac{a(a_1 - a_2 - c_1)}{\eta} + aa_2 \frac{\log \eta}{\eta} + \tilde{c}_3,$$
$$P = b_1\eta + b_2 \log \eta + \tilde{c}_4,$$

where $\tilde{c}_2 = c_2 + bc_1 + ba_2 - ba_1, \tilde{c}_3 = c_3 + aa_1 - aa_2 - ac_1, \tilde{c}_4 = c_4 - b_1$.

4. Example problems and numerical convergence tests

The scheme of algorithm testing is as follows: initially, we have obtained particular solutions of the Stokes and continuity equations for the exponential type of viscosity variation. Let us choose a domain, e.g., a rectangle in 2D case. We calculate values for velocity and pressure given by our analytical solution and take these values as the boundary conditions. Then, due to the uniqueness theorem, the solution of the boundary problem in the domain should coincide with our analytical solution. Let us compute the solution of the boundary problem by a numerical method. Comparison of the result with the exact analytical solution shows the quality of the numerical algorithm.

4.1. Exponentially varying viscosity

Consider a simple example of such flow in a rectangle $0 \leqslant x \leqslant x_{size}, 0 \leqslant y \leqslant y_{size}$. We assume that $\eta = ax + by + c$. We will mark the exact solution obtained in Section 2 as $v_{x,a}, v_{y,a}, P_a$. It is the solution of the boundary problem in the rectangle Ω with the following conditions at the boundary $\partial\Omega = \{x = 0, x = x_{size}, y = 0, y = y_{size}\}$:

$$v_y|_{\partial\Omega} = v_{y,a}, \quad v_x|_{\partial\Omega} = v_{x,a}.$$

Let us compute the velocity and pressure using the finite-difference scheme. The corresponding solution is marked as $v_{x,n}, v_{y,n}, P_n$. The deviation of these values from the exact solution $(v_{x,n} - v_{x,a}, v_{y,n} - v_{y,a}, P_n - P_a)$ is related with the error of the numerical scheme. We calculate the relative errors of three types: L_∞, L_1, L_2 for different viscosity contrasts , i.e. different values of the coefficients a, b. We test the program Stokes2D-variable-viscosity1 from [10]. The results are presented in Fig. 1-6. Namely, figures 1-3 correspond to low viscosity contrast, Figures 4-6 — to high viscosity contrast. Particularly, Fig. 1 and Fig. 4 show pressure and velocity components distributions. Fig. 2 and Fig. 5 characterize the viscosity and the density distributions. Fig. 3 and Fig. 6 contain plots of relative errors via the grid resolutions in logarithmic scale. The viscosity contrast, i.e. the values of the coefficients in the expression for the viscosity, is determined by the given values of the viscosity at three rectangle corners. The value of the viscosity at the initial rectangle corner is 1, η_2, η_3 are the values of the viscosity at two adjacent corners. For all figures, “n” means “numerical solution”, “a” means “analytical solution” (benchmark).

For the case of exponentially varying viscosity, we made calculations for the following system parameters:

$$C = \eta_1, a = (\log(\eta_3) - \log(\eta_1))/x_{size},$$
$$b = (\log(\eta_2) - \log(\eta_1))/y_{size},$$
$$\eta = C \exp{(ax + by)},$$
$$\rho = \beta_1\eta + \beta_2$$
$$x_{size} = y_{size} = 1,$$
$$G_x = 10, G_y = 10,$$
$$\eta_1 = 1, \beta_1 = 1, \beta_2 = 3 \times 10^3,$$

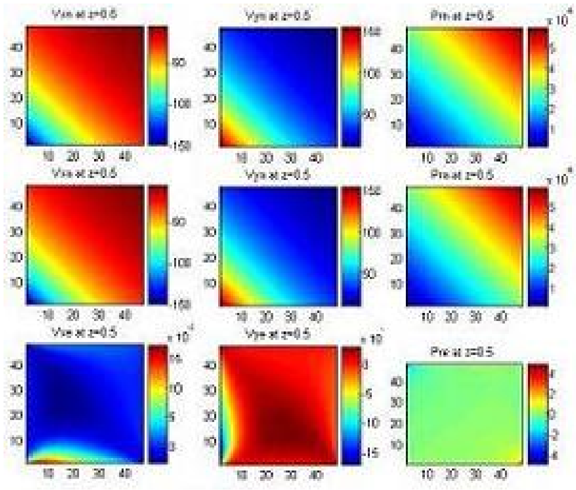

FIG. 1. Distribution of v_x, v_y and P; 2D case, exponentially varying viscosity, low viscosity contrast ($\eta_2 = \eta_3 = 5$).

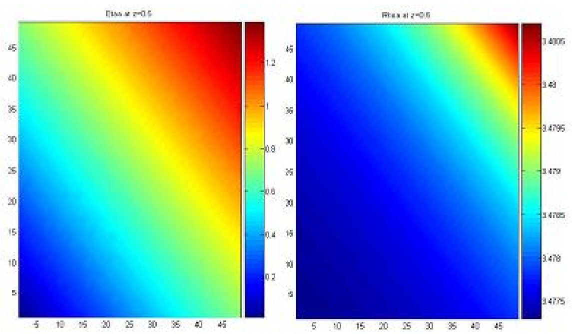

FIG. 2. Distribution of viscosity η and density ρ; 2D case, exponentially varying viscosity, low viscosity contrast ($\eta_2 = \eta_3 = 5$).

One can see that there is rather high accuracy for the numerical approach. Figures 1-3 corresponds to the case of low viscosity contrast, figures 4-6 — to the case of high viscosity contrast. We observe the conventional situation — L_∞-error is the largest among the considered errors norms, and L_1-error and L_2-error are similar. The calculations show that one has good convergence of the numerical scheme for small viscosity contrast, but it is not so for high viscosity contrast (compare Fig. 3 and Fig. 6).

5. Conclusion

Numerical analysis of geophysical flows presents many difficulties. It is related with complex dependence of material parameters on spatial coordinates. Different schemes of numerical calculations are suggested. To establish the quality of suggested approach it is possible to compare the results of different numerical methods. More reliable examination of the approach is given by the comparison with the exact solution of the problem, similar to the considered one. For this purpose, one needs such a benchmark solution. In the present paper, we suggest a benchmark solution for the Stokes equation coupled with the continuity equation where the viscosity is exponentially dependent upon the spatial Cartesian coordinates. Comparison of the numerical result with this exact solution allows us to determine the order of convergence, the quality of discretization, etc.

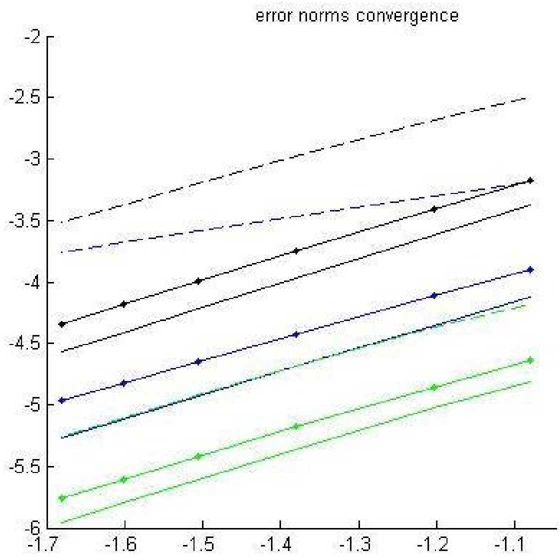

FIG. 3. Logarithm of the relative error via logarithm of the grid step; 2D case, exponentially varying viscosity, low viscosity contrast ($\eta_2 = \eta_3 = 5$); blue line - pressure, green - v_x, black - v_y; line - L_1-error, dashed line - L_∞-error, line with dots - L_2-error.

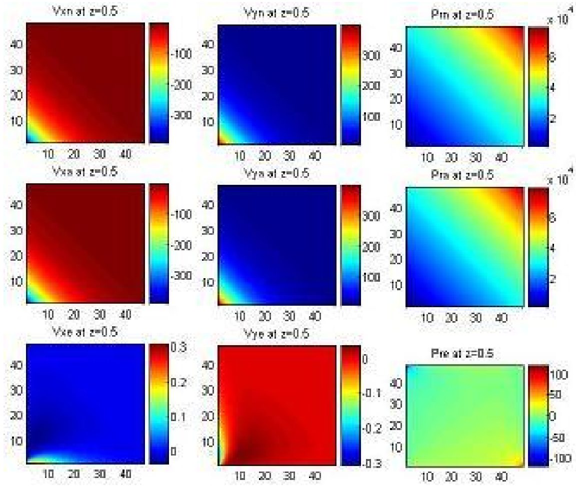

FIG. 4. Distribution of v_x, v_y and P; 2D case, exponentially varying viscosity, high viscosity contrast ($\eta_2 = \eta_3 = 100$).

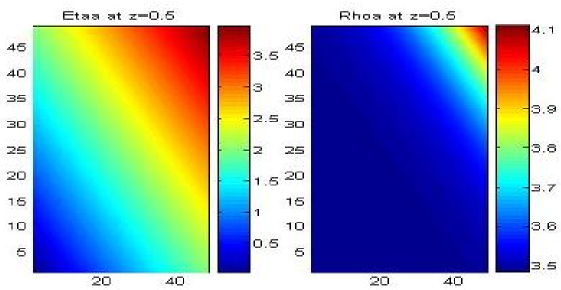

FIG. 5. Distribution of viscosity η and density ρ; 2D case, exponentially varying viscosity, high viscosity contrast ($\eta_2 = \eta_3 = 100$).

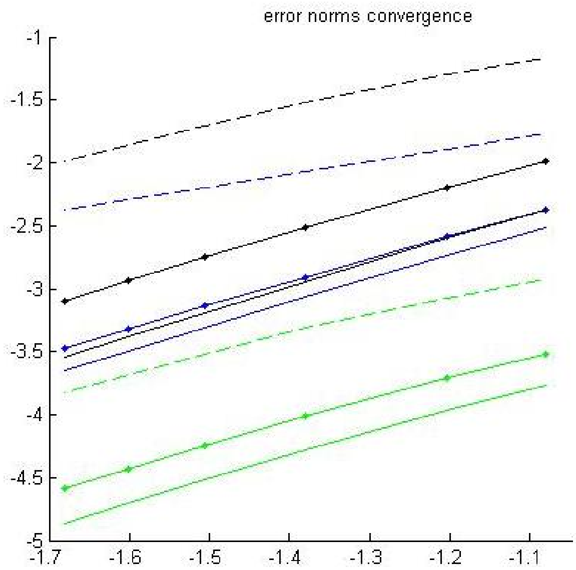

FIG. 6. Logarithm of the relative error via logarithm of the grid step; 2D case, exponentially varying viscosity, high viscosity contrast ($\eta_2 = \eta_3 = 100$); blue line - pressure, green - v_x, black - v_y; line - L_1-error, dashed line - L_∞-error, line with dots - L_2-error.

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