Solving PDE's with FEniCS

Advection

Chapter 15

Introduction to

Automated Modeling

with FEniCS

by L. Ridgway Scott

Many models balance advection and diffusion.

The basic advection-diffusion equation in a domain Ω is

$$-\epsilon\Delta u + \boldsymbol{\beta}\cdot\nabla u = f \text{ in } \Omega \tag{1}$$

where $\boldsymbol{\beta}$ is a vector-valued function indicating the advection direction.

Assume that we have boundary conditions

$$\begin{aligned} u &= g \text{ on } \Gamma \subset \partial\Omega && \text{(Dirichlet)} \\ \frac{\partial u}{\partial n} &= 0 \text{ on } \partial\Omega\backslash\Gamma && \text{(Neumann)} \end{aligned} \tag{2}$$

Neumann condition consistent with solution not changing much near boundary.

Posing Boundary Conditions

In advection-diffusion model, quantity u is advected in direction of $\boldsymbol{\beta}$.

- There are in-flow and out-flow parts of boundary.
- In-flow characterized by $\boldsymbol{\beta} \cdot \mathbf{n} < 0$ on Γ.

Specify u on Γ via $u = g_D$ on $\Gamma \subset \partial\Omega$

Out-flow boundary condition often requires modeling.

If behavior unknown at out-flow, best to do something neutral.

Posing Boundary Conditions

Suppose that we do nothing, in the sense that we

- use the variational space V defined for the Poisson problem
- then use the affine variational approach for inhomogeneous boundary conditions to define u,
- with $g_N = 0$ since we do not know how to specify g_N.

This corresponds to the boundary condition

$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega\backslash\Gamma. \tag{3}$$

Variational Formulation of advection-diffusion

Defining the variational form for advection-diffusion:

as before, using the three-step recipe, we define

$$\begin{aligned} a(u,v) &= \int_\Omega \nabla u(\mathbf{x}) \cdot \nabla v(\mathbf{x})\, d\mathbf{x} \\ b(u,v) &= \int_\Omega \big(\boldsymbol{\beta}(\mathbf{x}) \cdot \nabla u(\mathbf{x})\big) v(\mathbf{x})\, d\mathbf{x}. \end{aligned} \tag{4}$$

Alternative formulation: integrate by parts in the advection term.

Both forms are continuous on $H^1(\Omega)$.

What about coercivity?

Consider coercivity of the bilinear form

$$a_\beta(u,v) = \epsilon\, a(u,v) + b(u,v).$$

Since we already know that $a(\cdot,\cdot)$ is coercive on

$$V = \left\{ v \in H^1(\Omega) \;:\; v = 0 \text{ on } \Gamma \right\},$$

suffices to determine conditions under which

$$b(v,v) \geq 0 \text{ for all } v \in V.$$

Then

$$a_\beta(v,v) = \epsilon\, a(v,v) + b(v,v) \geq \epsilon\, a(v,v) \geq c\epsilon \left\| v \right\|_{H^1}^2 .$$

Positivity of the advection form

We again invoke the divergence theorem:

$$\begin{aligned}\oint_{\partial\Omega} u\,v\,\boldsymbol{\beta}\cdot\mathbf{n}\,ds &= \int_\Omega \nabla\cdot\left(u\,v\,\boldsymbol{\beta}\right)d\mathbf{x}\\ &= \int_\Omega u\boldsymbol{\beta}\cdot\nabla v + v\boldsymbol{\beta}\cdot\nabla u + u\,v\,\nabla\cdot\boldsymbol{\beta}\,d\mathbf{x},\end{aligned} \tag{5}$$

since $\nabla\cdot(w\boldsymbol{\beta}) = (\nabla w)\cdot\boldsymbol{\beta} + w\nabla\cdot\boldsymbol{\beta}$. In particular,

$$b(u,v) + b(v,u) = \oint_{\partial\Omega} u\,v\,\boldsymbol{\beta}\cdot\mathbf{n}\,ds - \int_\Omega u\,v\,\nabla\cdot\boldsymbol{\beta}\,d\mathbf{x}. \tag{6}$$

From (6), we have

$$2b(v,v) = \oint_{\partial\Omega} v^2\boldsymbol{\beta}\cdot\mathbf{n}\,ds - \int_\Omega v^2\nabla\cdot\boldsymbol{\beta}\,d\mathbf{x}. \tag{7}$$

Define

$$\begin{aligned}\Gamma_0 &= \{x \in \partial\Omega \;:\; \boldsymbol{\beta}(\mathbf{x}) \cdot \mathbf{n} = 0\}\,, \\ \Gamma_\pm &= \{x \in \partial\Omega \;:\; \pm\boldsymbol{\beta}(\mathbf{x}) \cdot \mathbf{n} > 0\}\,.\end{aligned} \tag{8}$$

An important special case is when

$\boldsymbol{\beta}$ is velocity in an **incompressible** fluid,

meaning $\nabla\cdot\boldsymbol{\beta} = 0$.

Think of β as solution of Stokes equations.

In the case $\nabla\cdot\boldsymbol{\beta} = 0$, (7) simplifies to

$$2b(v,v) = \oint_{\Gamma_-\cup\Gamma_+} v^2\boldsymbol{\beta}\cdot\mathbf{n}\,ds \geq \oint_{\Gamma_-} v^2\boldsymbol{\beta}\cdot\mathbf{n}\,ds, \qquad (9)$$

since, by definition,

$$\oint_{\Gamma_+} v^2\boldsymbol{\beta}\cdot\mathbf{n}\,ds \geq 0.$$

Suppose that $\Gamma_- \subset \Gamma$, meaning we impose Dirichlet boundary conditions on all of Γ_-.

Then $b(v,v) \geq 0$ for all $v \in V$,

and thus $a_\beta(\cdot,\cdot)$ is coercive on V.

In this case, u can be characterized uniquely via

$$u \in V \text{ satisfies } a_\beta(u,v) = (f,v)_{L^2(\Omega)} \quad \forall v \in V. \tag{10}$$

If $\nabla\cdot\boldsymbol{\beta} \leq 0$, coercivity of $a_\beta(\cdot,\cdot)$ again follows provided $\Gamma_- \subset \Gamma$.

But for more general $\boldsymbol{\beta}$, no guarantees can be made.

Now we consider an example for the problem (1):

$$\begin{aligned} -\epsilon\Delta u + \boldsymbol{\beta}\cdot\nabla u &= f \text{ in } \Omega \\ u &= g \text{ on } \Gamma. \end{aligned}$$

Let $\Omega = [0,1]^2$ and $\boldsymbol{\beta} = (1,0)$. Note that $\nabla\cdot\boldsymbol{\beta} = 0$.

An example

Let u_ϵ denote the solution of (1), and in the case that $\epsilon \to 0$, we denote the limiting solution by u_0 (if it exists).

We can solve (1) with $\epsilon = 0$ formally for a possible limit u_0 via

$$u_0(x, y) = \int_0^x f(s, y)\, ds + u_0(0, y). \tag{11}$$

Note that

$$\Gamma_- = \{(0, y) \;:\; y \in [0, 1]\}\,, \quad \Gamma_+ = \{(1, y) \;:\; y \in [0, 1]\}\,,$$

$$\Gamma_0 = \{(x, 0) \;:\; x \in [0, 1]\} \cup \{(x, 1) \;:\; x \in [0, 1]\}\,.$$

Variational problem (10) well posed provided $\Gamma_- \subset \Gamma$ (and provided $\epsilon > 0$).

Asymptotic solution

Then (11) implies that the likely limit would be

$$u_0(x,y) = \int_0^x f(s,y)\,ds + g(0,y). \qquad (12)$$

For example, if $f \equiv 1$, then

$$u_0(x,y) = x + g(0,y) \quad \text{for all} \quad x,y \in [0,1]^2.$$

This solution persists for $\epsilon > 0$ if, for example, $g(x,y) = a + by$, since $\Delta u_0 = 0$.

However, we need to pick the right boundary conditions if we want to get this solution.

Boundary conditions

If we expect to converge to the limit

$$u_0(x,y) = x + g(y) = x + a + by,$$

then boundary conditions should hold on u_0.

We assume that $u_0(0,y) = g(y)$ is imposed on Γ_-.

But on Γ_+, we have $(u_0)_{,x}(1,y) = 1$, so we would need inhomogeneous Neumann data there.

On Γ_0, we have $(u_0)_{,y}(x,0) = g'(0) = b$ and $(u_1)_{,y}(x,0) = g'(1) = b$.

So inhomogeneous Neumann data needed there, too.

Asymptotic solution

On the other hand, a Neumann condition $\frac{\partial u_0}{\partial x}(1, y) = 0$ holds if $f(1, y) = 0$, e.g., if $f(x, y) = 1 - x$.

Then

$$u_0(x, y) = x - \tfrac{1}{2}x^2 + g(0, y)$$

when $\epsilon = 0$.

If in addition, $\frac{\partial g}{\partial y}(0, 0) = \frac{\partial g}{\partial y}(0, 1) = 0$, then u_0 satisfies a Neumann condition on the top and bottom of $\Omega = [0, 1]^2$.

For example, we can take

$$g(x, y) = y^2\left(1 - \frac{2}{3}y\right). \tag{13}$$

Appropriate natural boundary conditions

In this case, we take $\Gamma = \Gamma_-$ and

$$u_0(x,y) = x - \tfrac{1}{2}x^2 + y^2\left(1 - \frac{2}{3}y\right). \qquad (14)$$

When ϵ is small, u_ϵ should be a small perturbation of this.

From Table 1, we see that indeed this is the case.

But if we also take $\Gamma_+ \subset \Gamma$ then we potentially obtain a constraint.

Compuational data

degree	mesh number	ϵ	$\epsilon^{-1}\|u_\epsilon - u_0\|_{L^2(\Omega)}$
4	8	1.0e+00	0.27270
4	8	1.0e-01	0.71315
4	8	1.0e-02	0.86153
4	8	1.0e-03	0.87976
4	8	1.0e-04	0.88172
4	8	1.0e-05	0.88190
4	8	1.0e-06	0.88191
4	8	1.0e-07	0.88192
4	8	1.0e-08	0.88192

Table 1: The diffusion advection problem (1)–(2) defines u_ϵ. u_0 is given in (14).

Advection equation code

Code to generate the data in Table 1.

```
# Define boundary condition
gee = Expression("x[1]*x[1]*(1.0-(2.0/3.0)*x[1])")
uex = Expression("(x[0]-(1.0/2.0)*x[0]*x[0])+ \
                  (x[1]*x[1]*(1.0-(2.0/3.0)*x[1]))")
bee = Constant((1.0,0.0))
bc = DirichletBC(V, gee, boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("1.0-x[0]")
a = (acoef*inner(grad(u), grad(v))+inner(bee,grad(u))*v)*dx
L = f*v*dx

# Compute solution
u = Function(V)
solve(a == L, u, bc)
```

A constraint

Equation (12) implies $g(1,y) = \int_0^1 f(s,y)\,ds + g(0,y)$, i.e.,

$$\int_0^1 f(s,y)\,ds = g(1,y) - g(0,y) \text{ for all } y \in [0,1]. \qquad (15)$$

If the data does not satisfy the constraint (15), we might expect some sort of boundary layer for $\epsilon > 0$.

In the case that g is given in (13) and $f(x,y) = 1 - x$, such a constraint holds, and we see in Figure 1(right) that there is a sharp boundary layer for $\epsilon = 0.001$.

For $\epsilon = 0.1$, Figure 1(left) shows that the solution deviates from u_0 over a broader area.

Boundary layer

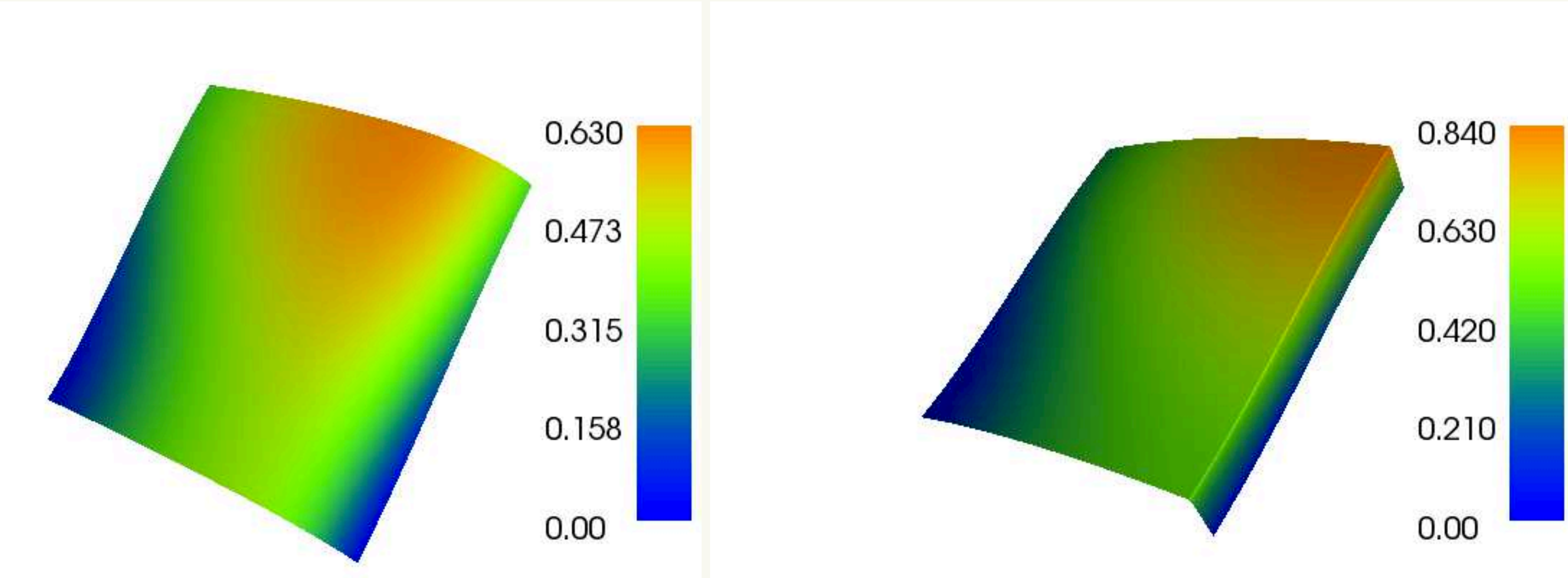

Figure 1: Diffusion-advection problem (1)–(2) with $\Gamma = \Gamma_- \cup \Gamma_+$ and g given in (13) and $f(x, y) = 1 - x$. Left: $\epsilon = 0.1$, u_ϵ computed using piecewise linears on a 100×100 mesh. Right: $\epsilon = 0.001$, u_ϵ computed using piecewise linears on a 1000×1000 mesh.

Numerical pollution

Middle ground ($\epsilon = 0.01$), boundary layer is still localized, Figure 2(left).

If we attempt to resolve this problem with too few grid points, as shown in Figure 2(right), then we get spurious oscillations on the scale of the mesh.

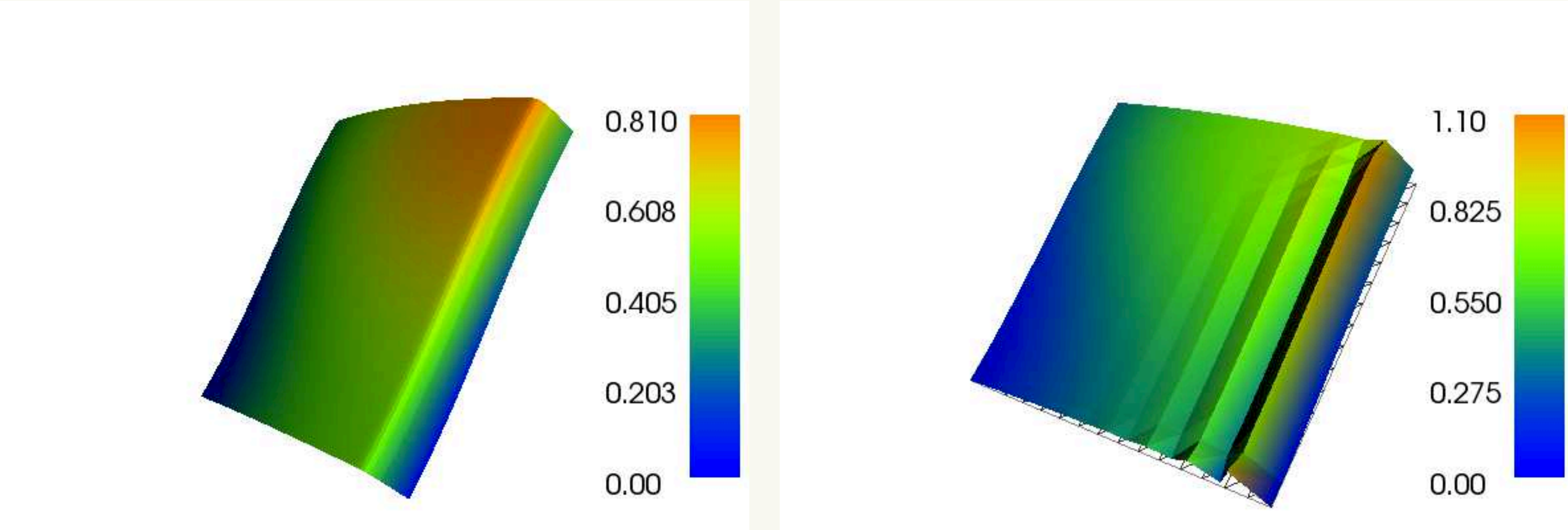

Figure 2: Diffusion-advection problem (1)–(2) with $\Gamma = \Gamma_- \cup \Gamma_+$ and g given in (13) and $f(x, y) = 1 - x$. Left: $\epsilon = 0.01$, u_ϵ computed using piecewise linears on a 100×100 mesh. Right: $\epsilon = 0.01$, u_ϵ computed using piecewise linears on a 15×15 mesh.

Wrong boundary conditions

Let us now ask the question:

what happens if $\Gamma_- \not\subset \Gamma$?

Take $\Gamma = \Gamma_+$ and consider (1)–(2) with g given in (13) and $f(x, y) = 1 - x$.

Numerical solutions for (10) depicted in Figure 3.

These look at first to be reasonable.

At least the case $\epsilon = 1.0$ looks plausible.

Reducing ϵ by a factor of 10 produces something like the boundary layer behavior we saw previously.

Wrong boundary conditions

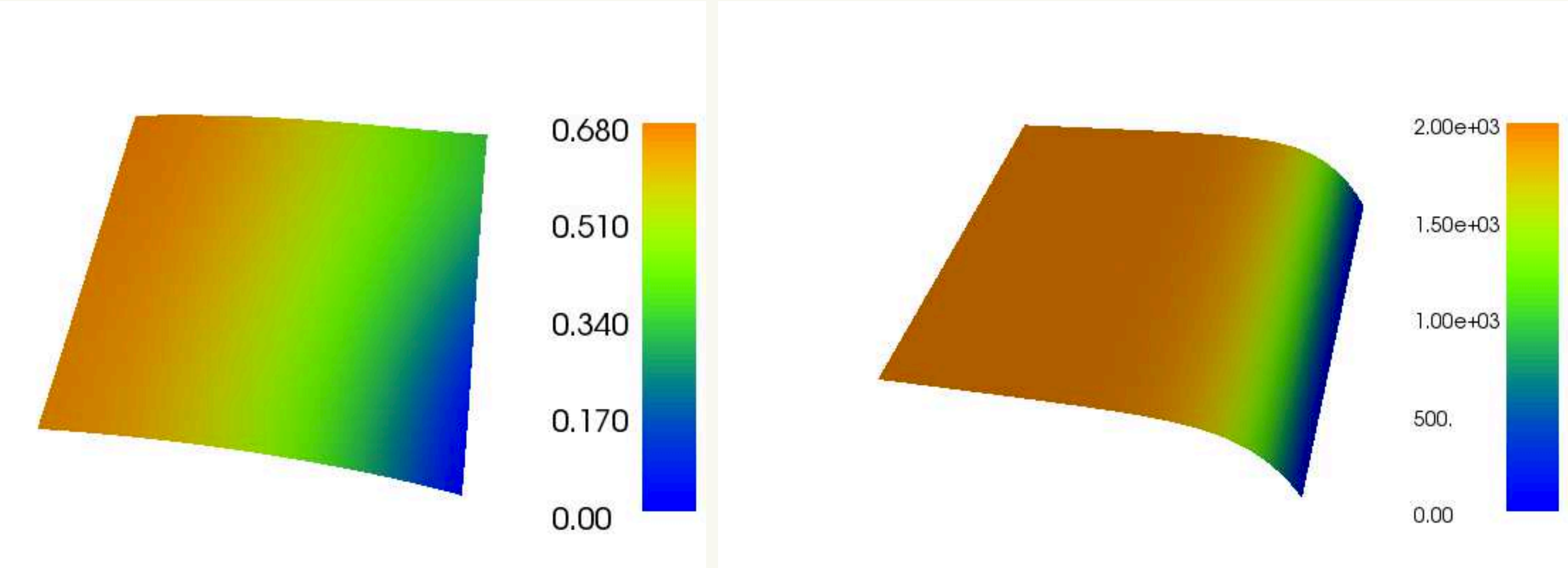

Figure 3: Diffusion-advection problem (1)–(2) with $\Gamma = \Gamma_+$ and g given in (13) and $f(x, y) = 1 - x$. Solution u_ϵ computed using piecewise linears on 100×100 mesh. Left: $\epsilon = 1.0$, Right: $\epsilon = 0.1$.

Don't be fooled

But look at the scale.

Solution is now extremely large.

If we continue to reduce ϵ (exercise) the solution size becomes disturbingly large.

Picking different orders of polynomials and values for ϵ gives random, spurious results.

Thus we conclude that the coercivity condition provides good guidance regarding how to proceed.

Crazy results

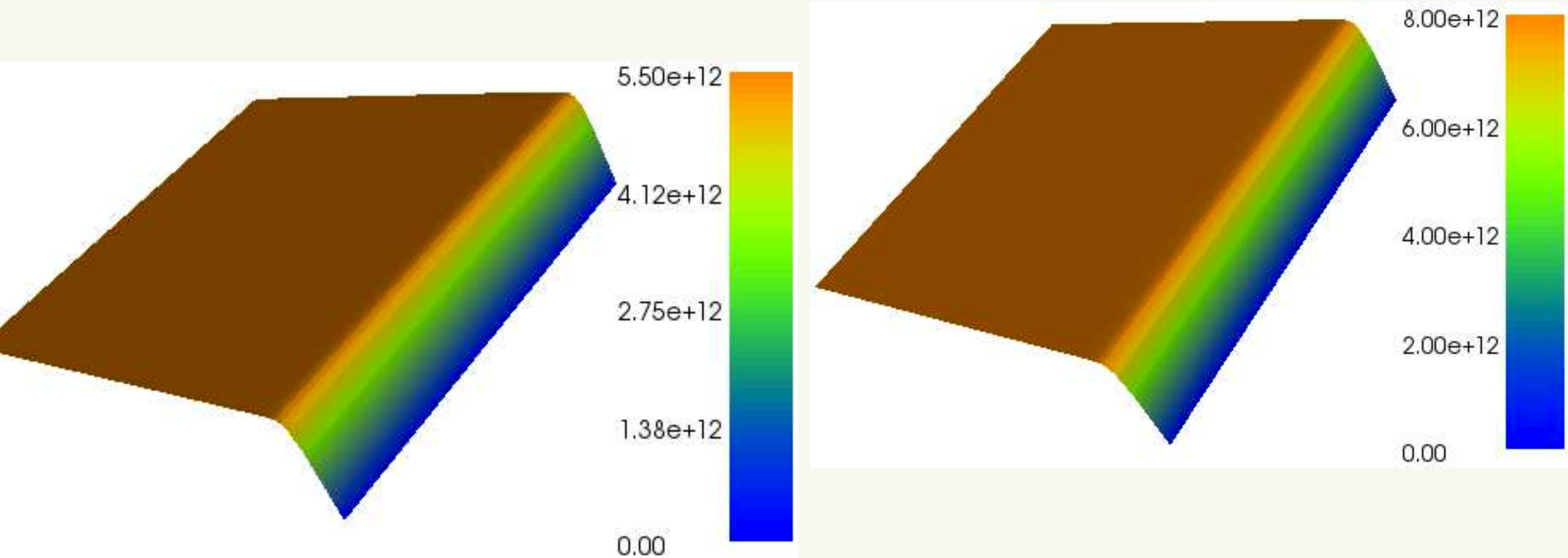

Figure 4: Diffusion-advection problem (1)–(2) with $\Gamma = \Gamma_+$ and g given in (13) and $f(x, y) = 1 - x$ and $\epsilon = 0.01$ on a 100×100. The solution u_ϵ was computed using piecewise linears (left) and piecewise quadratics (right).

Transport equation

In some cases, there is no natural diffusion in a system, and we are left with pure advection.

The resulting equation is often called a transport equation.

Such equations play a major role in non-Newtonian fluid models.

As a model equation of this type, we consider

$$\tau u + \boldsymbol{\beta} \cdot \nabla u = f \text{ in } \Omega. \tag{16}$$

Without a diffusion term, it is not possible to pose Dirichlet boundary conditions arbitrarily.

In the case where $\boldsymbol{\beta} \cdot \mathbf{n} = 0$ on $\partial\Omega$, the flow stays internal to Ω, and it has been shown [3, Proposition 3.7] that there is a unique solution $u \in L^2(\Omega)$ of (16) for any $f \in L^2(\Omega)$, provided that $\boldsymbol{\beta} \in H^1(\Omega)$.

Such results are extended in [1, 2] to the general case in which boundary conditions are posed on Γ_-.

The variational formulation of (16) involves the bilinear form

$$a_\tau(u, v) = \int_\Omega \tau uv + (\boldsymbol{\beta} \cdot \nabla u)v \, d\mathbf{x}. \tag{17}$$

In this case, u can be characterized uniquely via

$$u \in V \text{ satisfies } a_\tau(u, v) = (f, v)_{L^2(\Omega)} \quad \forall v \in V. \tag{18}$$

In our simple example with $\boldsymbol{\beta} = (1, 0)$, (16) can be written

$$\tau u(x, y) + u_{,x}(x, y) = f(x, y) \; \forall y \in [0, 1].$$

Fix $y \in [0, 1]$ and write $v(x) = e^{\tau x} u(x, y)$. Then

$$v'(x) = e^{\tau x}\big(\tau u(x, y) + u_{,x}(x, y)\big) = e^{\tau x} f(x, y),$$

so that

$$v(x) = v(0) + \int_0^x v'(s)\, ds = v(0) + \int_0^x e^{\tau s} f(s, y)\, ds.$$

Therefore

$$\begin{aligned} u(x,y) &= e^{-\tau x} v(x) \\ &= e^{-\tau x}\Big(u(0,y) + \int_0^x e^{\tau s} f(s,y)\, ds\Big) \\ &\forall (x,y) \in [0,1]\times[0,1]. \end{aligned} \tag{19}$$

For example, if we take $f(x,y) = e^{-\tau x}$, then $u(x,y) = g(y) + xe^{-\tau x}$, where g represents the Dirichlet data posed on $\Gamma = \Gamma_-$.

We leave as an exercise the development of a code for this problem.

Transport equation code

Code to implement the transport problem

```
acoeff=3.0
# Define boundary condition
gee = Expression("x[1]*x[1]*(1.0-(2.0/3.0)*x[1])")
uex = Expression("(x[0]+(x[1]*x[1]*(1.0-(2.0/3.0)*x[1]))) \
                 *exp(-ac*x[0])",ac=acoef)
bee = Constant((1.0,0.0))
bc = DirichletBC(V, gee, boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("exp(-ac*x[0])",ac=acoef)
a = (acoef*u*v+inner(bee,grad(u))*v)*dx
L = f*v*dx

# Compute solution
u = Function(V)
solve(a == L, u, bc)
```

Right boundary conditions

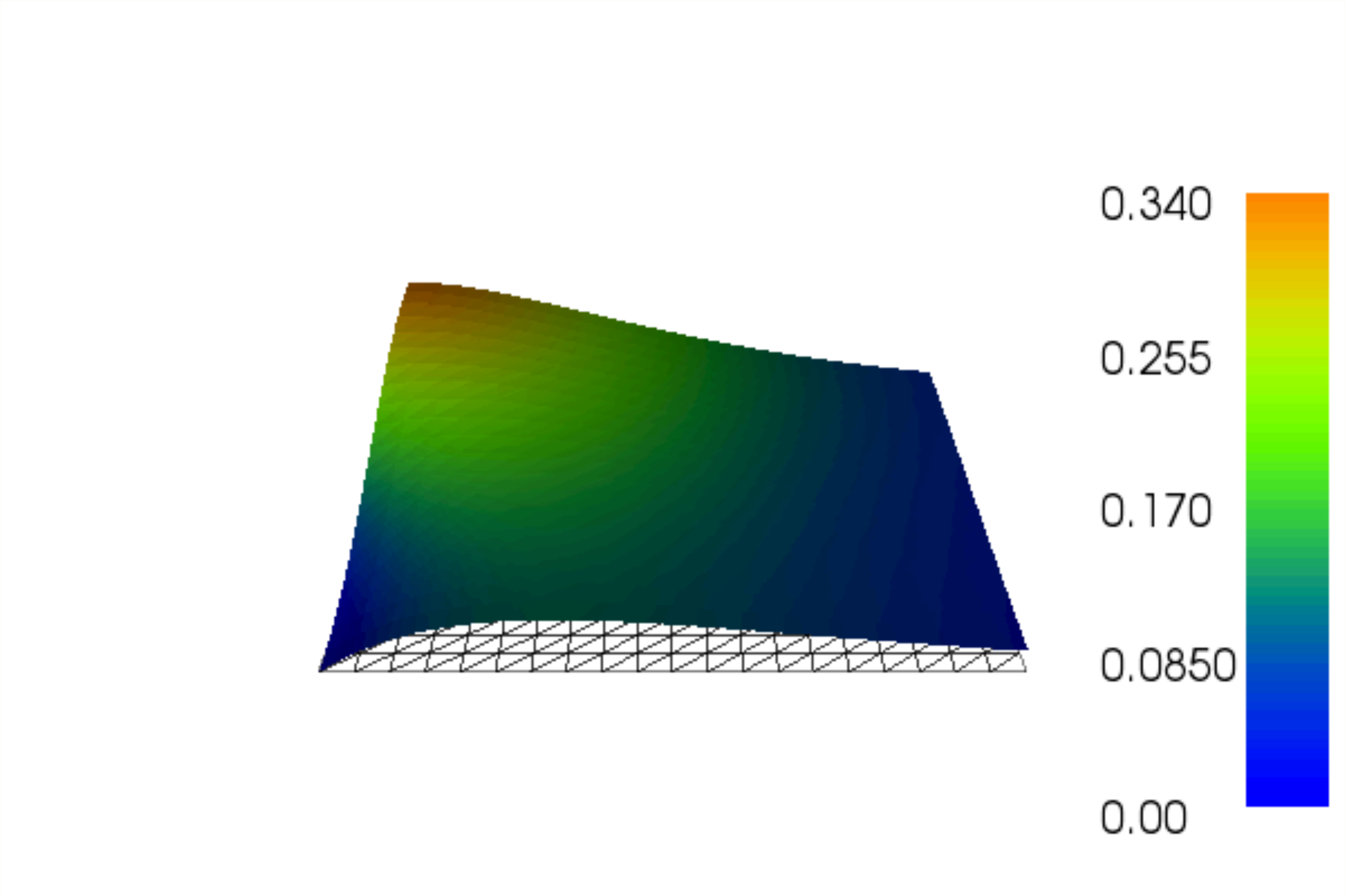

Figure 5: Transport problem with $\tau = 3.0$, with $f = e^{-\tau x_1}$, computed using piecewise linears on a 20×20 mesh. The boundary data g given in (13) was imposed on Γ_-.

Wrong boundary conditions

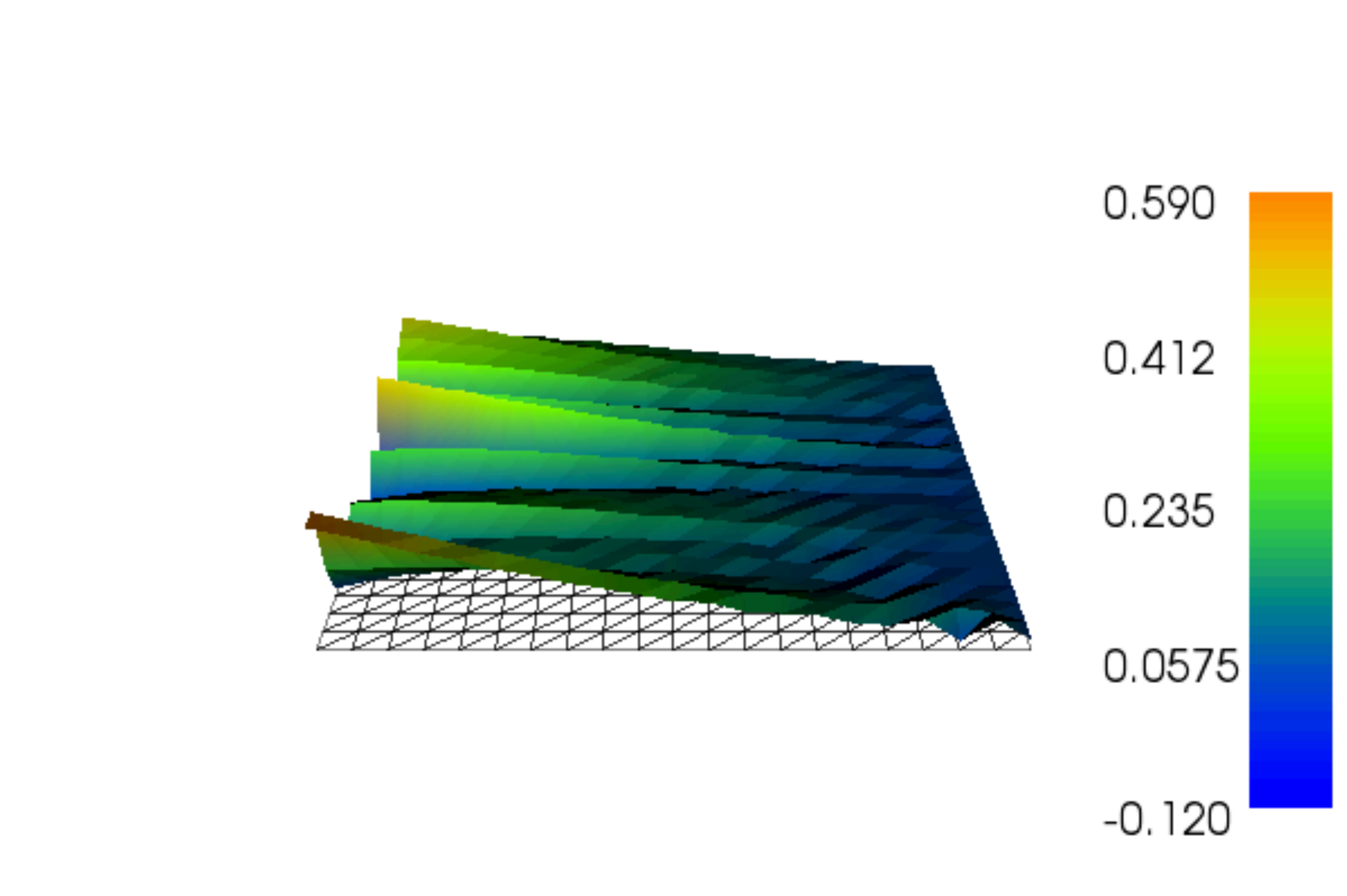

Figure 6: Transport problem with $\tau = 3.0$, with $f = e^{-\tau x_1}$, computed using piecewise linears on a 20×20 mesh. The boundary data g given in (13) was imposed on Γ_+.

References

[1] J.-M. Bernard. Steady transport equation in the case where the normal component of the velocity does not vanish on the boundary. *SIAM Journal on Mathematical Analysis*, 44(2):993–1018, 2012.

[2] Jean-Marie Bernard. Solutions in H^1 of the steady transport equation in a bounded polygon with a full non-homogeneous velocity. *Journal de Mathématiques Pures et Appliquées*, 107(6):697–736, 2017.

[3] V. Girault and L. Ridgway Scott. Analysis of a two-dimensional grade-two fluid model with a tangential boundary condition. *J. Math. Pures Appl.*, 78:981–1011, 1999.