Heterogeneous coupling for implicitly described domains

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1 Introduction

Many applications in physics, biology or chemistry exhibit complex geometrical shapes. Often these models feature partial differential equations (PDEs) on the complex shaped domain and its surface. At the same time the domain might be time-dependent, e.g. in cell biology the shape of a cell depends on its internal state and couples back to the cell metabolism, cf. [12]. Modern imaging techniques yield high resolution data of microscopic structures and thus allow us to exploit direct simulations.

Constructing suitable meshes for complex geometries is a very involved task, thus methods to decouple the computational mesh from the geometry are of great interest. In the context of Fictitious Domain Methods a wide range of methods was developed; we want to mention explicitly the Unfitted Finite Element Method [2, 13, 4], which we build upon. These methods formulate the original problem as a problem embedded in a larger domain. Different ways of incorporating the, now internal, boundary conditions are described in the literature. Examples for applications to coupled problems can be found using XFEM [9, 10], or using fictitious domain and mortar methods [1]. Many of these methods have been developed for engineering applications and are not directly applicable to biological problems as certain processes, e.g. topology changes can not be captured. An alternative class of methods uses implicit domain descriptions as level sets [17], or phase-field models [5, review paper]. Both approaches have been applied to coupled problems (e.g. [6, 18]), but due to the diffusive representation of the coupling interface these methods can lead to numerical artifacts, including spurious fluxes.

In this work we present a new approach to incorporate processes on manifolds in a heterogeneous domain-decomposition framework for implicitly described geometries. Although using a level set formulation, we avoid a diffuse coupling interface by utilizing an explicit reconstruction. It uses concepts of the Unfitted Finite Element Method and can be directly applied to image data.

Outline. The paper is structured as follows. In section 2 we discuss how domains can be described implicitly and in the following section we introduce the model problem. Section 4 describes the numerical scheme, starting with the Unfitted Discontinuous Galerkin approach for volume equations and then presenting a consistent approach for equations on the surface as well as the way of imposing coupling conditions. Finally, a numerical example is discussed in section 5.

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2 Implicitly described domains

For each $t \in [0,T]$, $T > 0$, let $\Omega(t) \subset \mathbb{R}^n$ be a Lipschitz bounded domain and $\Gamma(t)$ its boundary, with ν denoting the outward pointing unit normal vector field to $\Gamma(t)$.

By embedding $\Omega(t)$ in a larger stationary domain $\hat{\Omega}$, it is possible to describe $\Omega(t)$ using the so-called level set approach [14]. It captures the geometric information and motion of a moving interface from an Eulerian point of view in terms of a level set function and an associated PDE. A level set function is a scalar function $\Phi(x,t)$ defined in $\hat{\Omega} \times [0,T]$ with

$$\Phi(x,t) \begin{cases} < 0 & \text{for } x \in \Omega(t), \\ = 0 & \text{for } x \in \Gamma(t), \\ > 0 & \text{else,} \end{cases}$$

like illustrated in Figure 1. For each t the interface $\Gamma(t)$ corresponds to the zero level set $\Phi^{-1}(0) := \{x \in \hat{\Omega} \mid \Phi(x,t) = 0\}$. $\Phi(x,t)$ satisfies the level set advection equation

$$\Phi_t + \mathbf{v} \cdot \nabla \Phi = 0,$$

where $\mathbf{v}(x,t)$ is a velocity field corresponding to the evolution of $\Omega(t)$ and $\Gamma(t)$.

The level set approach allows for an elegant treatment of complex geometrical morphologies with potential topology changes in a fully implicit way, as discrete versions of Φ can be defined using a fixed grid on $\hat{\Omega}$. It is convenient to choose an appropriate $\hat{\Omega}$ which allows to use a simple Cartesian grid.

In this paper we only consider static domains, i.e. $\mathbf{v} \equiv 0$. Eulerian formulations of PDEs on moving domains contain additional terms corresponding to the transport of information induced by domain movement, the so-called material derivatives. The numerical schemes we present in section 4 are extended accordingly by appropriate transport terms.

3 Model problem

Let u_1 and u_2 denote the concentrations of two scalar quantities on a static domain Ω and its surface Γ, respectively. Conservation of these quantities with a diffusive flux $-\mathscr{D}_1 \nabla u_1$ in Ω and a diffusive surface flux $-\mathscr{D}_2 \nabla_\Gamma u_2$ together with an additional reactive process on Γ leads to the model problem we want to consider. Given some initial values $u_1(\cdot,0)$ and $u_2(\cdot,0)$, it reads

$$\partial_t u_1 = \nabla \cdot (\mathscr{D}_1 \nabla u_1) \qquad \text{in} \quad \Omega \times (0,T], \tag{1a}$$

$$\partial_t u_2 = \nabla_\Gamma \cdot (\mathscr{D}_2 \nabla_\Gamma u_2) + r_2\big(u_1|_\Gamma, u_2\big) \qquad \text{on} \quad \Gamma \times (0,T], \tag{1b}$$

$$\mathscr{D}_1 \nabla u_1 \cdot \nu = r_1\big(u_1|_\Gamma, u_2\big) \qquad \text{on} \quad \Gamma \times (0,T]. \tag{1c}$$

Here, ∇_Γ denotes the tangential surface gradient as well as the induced surface divergence. $\mathscr{D}_1$ and $\mathscr{D}_2$ are the particular volume and surface diffusivity tensors, i.e. $\mathscr{D}_2$ maps the tangent space of Γ into itself at every point. r_1 together with r_2 are potentially nonlinear terms which couple the processes in Ω and Γ. For example, they could describe transitions between u_1 and u_2. The coupling in equation (1a) is due to its Robin-like boundary condition (1c), whereas r_2 appears as a standard surface reaction term in equation (1b).

4 Heterogeneous coupling

We propose a new numerical scheme for solving problems like model problem (1). It is based on the Unfitted Discontinuous Galerkin method (UDG) for solving PDEs in Ω and a level set based extension to surface PDEs. The method of lines [16] is used to split spatial and temporal operators. A semi-discretization in space yields: Find $(u_{1,h}, u_{2,h}) \in L^2(0,T;V_{1,h}) \times L^2(0,T;V_{2,h})$ such that for each $t \in (0,T]$

$$\begin{aligned} t_{\text{vol}}(u_{1,h}, v_{1,h}, t) + a_{\text{vol}}(u_{1,h}, v_{1,h}, t) + c_1(u_{1,h}, u_{2,h}, v_{1,h}, t) = 0 \quad \forall v_{1,h} \in V_{1,h}, \\ t_{\text{sur}}(u_{2,h}, v_{2,h}, t) + a_{\text{sur}}(u_{2,h}, v_{2,h}, t) + c_2(u_{1,h}, u_{2,h}, v_{2,h}, t) = 0 \quad \forall v_{2,h} \in V_{2,h}, \end{aligned} \tag{2}$$

where $V_{1,h}$ and $V_{2,h}$ denote discrete function spaces. The operators t_{vol} and t_{sur} correspond to the two time derivatives $\partial_t u_1$ and $\partial_t u_2$ in problem (1). The elliptic diffusion terms of equations (1a) and (1b) are contained in the operators a_{vol} and a_{sur}, respectively, and c_1 and c_2 are coupling operators which correspond to the terms r_1 and r_2. To get a fully discrete scheme, different time discretization schemes can be used.

Bulk discretization: The Unfitted Discontinuous Galerkin method. To treat the bulk equations (1a, 1c), we consider the UDG method [4], which is a general approach for simulations on complicated domains. It uses the concepts of the Unfitted Finite Element Method [2, 13] and discretizes PDEs on an unfitted mesh, i.e. the domain boundary Γ is not resolved by the mesh. For an easy implementation, this so called *fundamental mesh* is chosen to be the same mesh as for the discrete level set function. Shape functions are defined on the unfitted mesh and their support is restricted to Ω. We use a Discontinuous Galerkin (DG) discretization. This allows to easily incorporate local mass conservation and to use higher order shape functions.

Based on the fundamental mesh $\mathscr{T}(\hat{\Omega}) := \{\hat{E}_0, \dots, \hat{E}_{M-1}\}$, a Finite Element mesh for domain Ω is defined by intersecting Ω and $\mathscr{T}(\hat{\Omega})$ (see Figure 1):

$$\mathscr{T}(\Omega) := \{E_n = \Omega \cap \hat{E}_n \mid \hat{E}_n \in \mathscr{T}(\hat{\Omega}),\ |E_n| > 0\}.$$

The elements E_n can be arbitrarily shaped and in general will not be convex. Using standard DG shape functions on $\mathscr{T}(\hat{\Omega})$ with their support restricted to the elements in $\mathscr{T}(\Omega)$, the resulting Finite Element space is defined by

$$V_{1,h} := \left\{ v \in L^2(\Omega) \;\middle|\; v|_{E_n} \in P_k \ \forall E_n \in \mathscr{T}(\Omega) \right\},$$

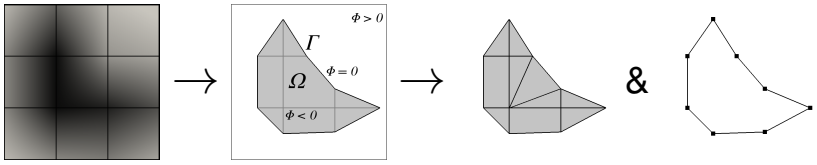

Fig. 1 Given the fundamental mesh $\mathscr{T}(\hat{\Omega})$ and a piecewise linear level set function Φ (left), the domain Ω and the Finite Element mesh $\mathscr{T}(\Omega)$ are defined. Local triangulations of its cells E_n and ∂E_n yield a partition of Ω into integration parts $\{E_{n,k}\}$ and a piecewise linear reconstruction of Γ.

P_k being the space of polynomial functions of degree k. $V_{1,h}$ is discontinuous on the internal skeleton $\Gamma_{\text{int}} := \{\gamma_{n,m} = \partial E_n \cap \partial E_m \mid E_n, E_m \in \mathscr{T}(\Omega),\ E_n \neq E_m,\ |\gamma_{n,m}| > 0\}$, with $|\gamma_{n,m}|$ denoting the codimension one volume of $\gamma_{n,m}$, but not on the external skeleton $\Gamma_{\text{ext}} := \{\gamma_n = \partial E_n \cap \partial\Omega \mid E_n \in \mathscr{T}(\Omega),\ |\gamma_n| > 0\}$. To each $\gamma_{n,m} = \gamma_{m,n}$, we assign unit normal vector fields $\mathbf{n}_{E_n} \equiv -\mathbf{n}_{E_m}$ and arbitrarily choose $\mathbf{n} := \mathbf{n}_{E_n}$. Using the DG formulation described in [15], the operators which result from eq. (1a) read:

$$t_{\text{vol}}(u_{1,h}, v_{1,h}, t) := \frac{d}{dt} \sum_{E_n \in \mathscr{T}(\Omega)} \int_{E_n} u_{1,h}\, v_{1,h}\, dV,$$

$$a_{\text{vol}}(u_{1,h}, v_{1,h}, t) := \sum_{\gamma_{n,m} \in \Gamma_{\text{int}}} \int_{\gamma_{n,m}} \varepsilon \langle (\mathscr{D}_1 \nabla v_{1,h}) \cdot \mathbf{n} \rangle [u_{1,h}] - \langle (\mathscr{D}_1 \nabla u_{1,h}) \cdot \mathbf{n} \rangle [v_{1,h}]\, ds$$
$$+ \sum_{E_n \in \mathscr{T}(\Omega)} \int_{E_n} (\mathscr{D}_1 \nabla u_{1,h}) \cdot \nabla v_{1,h}\, dV + \sum_{\gamma_{n,m} \in \Gamma_{\text{int}}} \frac{\sigma}{|\gamma_{n,m}|^\beta} \int_{\gamma_{n,m}} [u_{1,h}][v_{1,h}]\, ds.$$

Here, σ and β are appropriate stabilization parameters and $\varepsilon = \pm 1$. Furthermore, $[\cdot]$ denotes the jump of a function $v \in V_{1,h}$ on the interface between two adjacent elements E_n, E_m which is defined as $[v] := v|_{\partial E_n} - v|_{\partial E_m}$ and the average $\langle \cdot \rangle$ is defined as $\langle v \rangle := \frac{1}{2}\left(v|_{\partial E_n} + v|_{\partial E_m}\right)$.

Assembling the local stiffness matrix requires integration over the volume of each element E_n and different parts of its surface ∂E_n. As these mesh elements might exhibit very complicated shapes, quadrature rules based on interpolation functions are not directly applicable. Integation on the fundamental mesh also does not work, since shape functions are discontinuous. In order to guarantee accurate evaluation of integals in an efficient manner, quadrature rules for irregular shaped elements are constructed using a local triangulation of E_n. To do so, E_n is subdivided into a disjoint set $\{E_{n,k}\}_k$ of simple geometric objects, i.e. simplices and hypercubes. For each of these *integration parts* an efficient Gauss type quadrature rule is available. For a piecewise linear approximation of the level set function, the local triangulation can be efficiently constructed by applying a modified marching cubes algorithm [4].

Extension to surface equations. The pure surface part of model problem (1) without the coupling term r_2 reads

$$\partial_t u_2 = \nabla_\Gamma \cdot (\mathscr{D}_2 \nabla_\Gamma u_2) \quad \text{on} \quad \Gamma \times (0, T]. \tag{3}$$

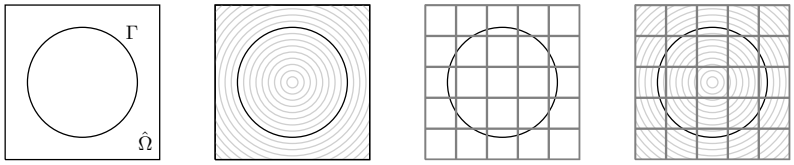

Fig. 2 From left to right: Surface Γ embedded into the larger level set domain $\hat{\Omega}$, Γ and some other level sets Γ_r of Φ, the same together with a Cartesian grid on $\hat{\Omega}$.

To treat this equation, we combine the DG method with an implicit surface Finite Element approach which was introduced in [7]. Similar to the method described in [7], we make use of the implicit level set description of Γ. The basic idea is to extend a surface diffusion equation like (3) and its solution to the whole level set domain $\hat{\Omega}$ by simultaneously formulating the $(n-1)$-dimensional PDE on all level surfaces of Φ. The resulting n-dimensional problem is solved using a DG discretization on an arbitrary triangulation of $\hat{\Omega}$. See also Figure 2. The solution of the original surface problem is then obtained by restricting the higher dimensional solution to Γ.

In particular, we use that we can partition $\hat{\Omega}$ into level surfaces

$$\Gamma_r := \left\{ x \in \hat{\Omega} \;\middle|\; \Phi(x) = r \right\}$$

with $\bigcup_{r\in(\Phi_{\min},\Phi_{\max})} \Gamma_r = \hat{\Omega}$, $\Phi_{\min} := \inf_{x\in\hat{\Omega}} \Phi(x)$, $\Phi_{\max} := \sup_{x\in\hat{\Omega}} \Phi(x)$. Note that $\Gamma = \Gamma_0$. First, we create a suitable extension $\mathscr{D}_2^{\Phi}$ of the surface diffusivity tensor $\mathscr{D}_2$ to the level set domain $\hat{\Omega}$, such that we do not have any diffusion normal to any level surface. In detail, $\mathscr{D}_2^{\Phi}$ is chosen such that $\mathscr{D}_2^{\Phi}\big|_{\Gamma} = \mathscr{D}_2$ and

$$\mathscr{D}_2^{\Phi} \nu^{\perp} \cdot \nu = 0 \quad \text{in} \quad \hat{\Omega} \times (0,T] \tag{4}$$

for every tangential vector $\nu^{\perp}$, where we now denote by ν the outward pointing unit normal vector field to every level surface. Then the elliptic surface differential operator ∇_{Γ} is extended to each level surface Γ_r yielding a differential operator ∇_{Φ}. Using these extensions, (3) is formulated on all level surfaces Γ_r. This results in the n-dimensional equation

$$\partial_t u_2 = \nabla_{\Phi} \cdot \left(\mathscr{D}_2^{\Phi} \nabla_{\Phi} u_2 \right) \quad \text{in} \quad \hat{\Omega} \times (0,T].$$

Assuming that the level set function Φ is differentiable and satisfies a non-degeneracy condition $\nabla\Phi \neq 0$ in $\hat{\Omega} \cup \partial\hat{\Omega}$, we can follow the approach from [7, Remark 3.3] and reformulate the extended tangential surface divergence operator ∇_{Φ}. This results in an equivalent equation

$$\partial_t u_2 |\nabla\Phi| = \nabla \cdot \left(\tilde{\mathscr{D}}_2^{\Phi} \nabla u_2 \right) \quad \text{in} \quad \hat{\Omega} \times (0,T], \tag{5}$$

with a modified diffusion tensor $\tilde{\mathscr{D}}_2^{\Phi} := |\nabla\Phi| \mathscr{D}_2^{\Phi} \mathscr{P}_{\Phi}$. At every point in $\hat{\Omega}$, $\mathscr{P}_{\Phi}$ is the operator which projects onto the tangent space of the corresponding level sur-

face. Equation (5) is a usual parabolic diffusion equation in $\mathbb{R}^n$ with a special mass density. In order to define a well-posed problem it has to be supplemented by initial values and an appropriate boundary condition for u_2 on $\partial\hat{\Omega}$. We choose initial values which are an arbitrary but continuous extension of the original initial values chosen for equation (1b) and use the natural no-flux boundary condition $\tilde{\mathscr{D}}_2^{\Phi}\nabla u_2 \cdot \nu_{\partial\hat{\Omega}} = 0$, with the outer unit normal $\nu_{\partial\hat{\Omega}}$. Note that the restricted solution on a particular level surface Γ_r only depends on the values of data on that surface as we do not have any diffusion in the normal direction due to equation (4). Therefore it is independent of the solutions on any other level surface. It can, however, be related to these solutions by the extensions of the data. Furthermore, it is not affected by the artificial boundary condition as long as Γ_r does not intersect $\partial\hat{\Omega}$. Further note that the solution on Γ, i.e. $u_2|_\Gamma$, solves equation (3).

The initial-boundary-value problem resulting from equation (5) can be discretized on the fundamental mesh $\mathscr{T}(\hat{\Omega})$ by usual grid-based numerical methods. Using the same DG formulation as for the volume part, we obtain:

$$t_{\text{sur}}(u_{2,h}, v_{2,h}, t) := \frac{d}{dt} \sum_{\hat{E}_n \in \mathscr{T}(\hat{\Omega})} \int_{\hat{E}_n} u_{2,h}\, v_{2,h}\, |\nabla\Phi|\, dV,$$

$$\begin{aligned} a_{\text{sur}}(u_{2,h}, v_{2,h}, t) := &\sum_{\hat{\gamma}_{n,m} \in \hat{\Gamma}_{\text{int}}} \int_{\hat{\gamma}_{n,m}} \varepsilon \left\langle \left(\tilde{\mathscr{D}}_2^{\Phi}\nabla v_{2,h}\right)\cdot\mathbf{n}\right\rangle [u_{2,h}] - \left\langle \left(\tilde{\mathscr{D}}_2^{\Phi}\nabla u_{2,h}\right)\cdot\mathbf{n}\right\rangle [v_{2,h}]\, ds \\ &+ \sum_{\hat{E}_n \in \mathscr{T}(\hat{\Omega})} \int_{\hat{E}_n} \left(\tilde{\mathscr{D}}_2^{\Phi}\nabla u_{2,h}\right)\cdot\nabla v_{2,h}\, dV + \sum_{\hat{\gamma}_{n,m} \in \hat{\Gamma}_{\text{int}}} \frac{\sigma}{|\hat{\gamma}_{n,m}|^{\beta}} \int_{\hat{\gamma}_{n,m}} [u_{2,h}][v_{2,h}]\, ds. \end{aligned}$$

Here, we choose the discrete function space

$$V_{2,h} := \left\{ v \in L^2(\hat{\Omega}) \;\middle|\; v|_{\hat{E}_n} \in P_k \;\forall \hat{E}_n \in \mathscr{T}(\hat{\Omega}) \right\},$$

and the jump $[\cdot]$ and average $\langle\cdot\rangle$ act on functions from $V_{2,h}$, targeting discontinuities that lie on the internal skeleton of $\mathscr{T}(\hat{\Omega})$, which is defined by

$$\hat{\Gamma}_{\text{int}} := \left\{ \hat{\gamma}_{n,m} = \partial\hat{E}_n \cap \partial\hat{E}_m \;\middle|\; \hat{E}_n, \hat{E}_m \in \mathscr{T}(\hat{\Omega}),\ \hat{E}_n \neq \hat{E}_m,\ |\hat{\gamma}_{n,m}| > 0 \right\}.$$

Explicit coupling of bulk and surface. The volume coupling operator c_1 results from the way DG formulations include boundary conditions of Robin type. For boundary condition (1c) we get

$$c_1(u_{1,h}, u_{2,h}, v_{1,h}, t) := -\sum_{\gamma_n \in \Gamma_{\text{ext}}} \int_{\gamma_n} r_1\left(u_{1,h}|_\Gamma, u_{2,h}|_\Gamma\right) v_{1,h}|_\Gamma\, ds.$$

The surface coupling operator c_2 is imposed directly along Γ by choosing

$$c_2(u_{1,h}, u_{2,h}, v_{2,h}, t) := -\sum_{\gamma_n \in \Gamma_{\text{ext}}} \int_{\gamma_n} r_2\left(u_{1,h}|_\Gamma, u_{2,h}|_\Gamma\right) v_{2,h}|_\Gamma\, ds,$$

such that the native surface reaction term r_2 from equation (1b) now acts like the lower order term in a Robin-like inner boundary condition. The integrals over each γ_n are efficiently evaluated using the local triangulation of the bulk discretization. In each time step, this results in a globally coupled block system $A = \begin{pmatrix} A_{vol} & C_1 \\ C_2 & A_{sur} \end{pmatrix}$, which can be solved fully coupled or using a Schwarz type iteration.

5 Numerical example and conclusion

We compute a problem from cell biology. Prior to cell division, the shape of a single yeast cell can be idealized as a circular domain $\Omega \subset \mathbb{R}^2$ whose surface Γ is the cell membrane. We use eq. (1) to model the intracellular pathway of a protein known as CDC42, where u_1 and u_2 denote its bulk and surface concentration. Diffusion driven instabilities lead to clustering of CDC42 on the membrane, which triggers the sprouting of a bud in areas of high concentration. The model uses coupling terms $r_2(u_1,u_2) := -r_1(u_1,u_2) := k_1 \cdot u_1 u_2^2 + k_2 \cdot u_1 u_2 - k_3 \cdot u_2$, $k_1 := 0.0036$, $k_2 := 0.0067$, $k_3 := 0.01733$, which describe transitions between CDC42 inside of the cell and on its membrane, and constant diffusivities $\mathscr{D}_1 := 10$, $\mathscr{D}_2 := 0.0025 =: \mathscr{D}_2^\Phi$.

In our simulation, we use a level set domain $\hat{\Omega} = [0,1]^2$ and a Cartesian fundamental mesh $\mathscr{T}(\hat{\Omega})$ which contains 32×32 elements. The cell Ω is positioned in the center of $\hat{\Omega}$. It is described by a level set function $\Phi(x) := \|x - (0.5,0.5)^T\| - 0.35$ which is approximated using Q1 Finite Elements on $\mathscr{T}(\hat{\Omega})$.

The discretization is done using polynomial degree $k = 1$. For bulk discretization we choose $\varepsilon = -1$, the Interior Penalty Galerkin scheme. For the surface discretization we use $\varepsilon = +1$, the Nonsymmetric Interior Penalty Galerkin scheme. The resulting semi-discretized problem (2) is solved using Newton's method for linearization and the fractional step θ-method [11] for time discretization. As shown in Figure 3, random generated initial values for u_1 and u_2 lead to the expected localization of u_2 on the membrane.

Conclusion. The proposed approach yields a unified setting for coupled volume and surface problems. The same infrastructure can be used to implement the discretization of both the volume and the surface part. Coupling conditions are handled explicitly along the surface in an efficient way without additional effort. At the same time we use an implicit description of the domain which makes the method completely independent of the problem's geometry. This level set based Eulerian formulation makes the approach a promising tool for biological problems, especially those which involve strongly evolving domains with potential topology changes.

Future topics may include the application to evolving domain problems or a thorough error analysis.

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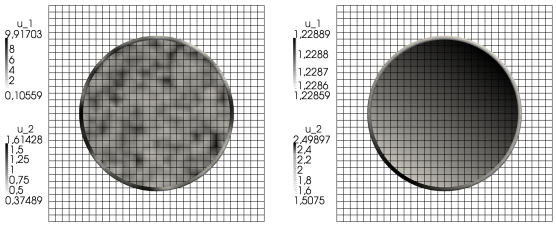

Fig. 3 Left: Initial values on a circular shaped domain Ω and its surface Γ. Right: Simulation result at final time $T = 500$, using polynomial degree $k = 1$ and time step $dt = 0.5$; note the localization of u_2 on Γ at the lower left.

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