

# Finite Element Convergence Studies of a Time-Dependent Test Problem Using COMSOL 5.1

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## Abstract

The finite element method (FEM) is a well known numerical method in solving partial differential equations (PDEs). All numerical methods inherently have error in comparison to the true solution of the PDE. Base on the FEM theory, the appropriate norm of this error is bounded and it can be estimated by the mesh size. One standard method to get an idea about the sensibility of the numerical solution is to do convergence studies on the method. More precisely, compare the results obtained from two consecutive mesh refinements. This comparison, then can be quantified using theory of FEM by obtaining the convergence order. In this paper we carry out convergence studies for the time-dependent parabolic test problem (the heat transfer equation) and investigate the effect of ODE solver on the behavior of the convergence of the method using commercial FEM software COMSOL 5.1.

**Keywords:** Parabolic PDE, heat transfer equation, method of lines (MOL), convergence study, mesh refinement.

## 1 Introduction

### 1.1 Time-Dependent PDEs

The time-dependent heat transfer equation is classical example of parabolic partial differential equation (PDE). The general form of this kind of problems is stated in (1)–(3) as

$$u_t - \nabla \cdot (D\nabla u) + a_0 u = f \quad \text{in } \Omega \text{ for } t_0 < t \leq t_{fin}, \quad (1)$$

$$\mathbf{n} \cdot (D\nabla u) = r \quad \text{on } \partial\Omega \text{ for } t_0 < t \leq t_{fin}, \quad (2)$$

$$u = u_{ini} \quad \text{in } \bar{\Omega} \text{ at } t = t_0, \quad (3)$$

where  $f(x, y)$  and  $r(x, y)$  are some given functions on the spatial domain  $\Omega \subset \mathbb{R}^d$  in  $d$  dimensions and its boundary  $\partial\Omega$ , respectively in timespan  $[t_0, t_f]$ . And  $u_{ini}$  being the initial value of  $u$  at  $t = t_0$ . More information on these kind of PDEs can be found in [1].

### 1.2 Method of Lines

One of the standard methods to solve the aforementioned time-dependent PDE is to discretize the spatial domain  $\Omega$ , to obtain system of ordinary differential equations (ODEs) for every grid point of discretized domain ( $\Omega_h$ ). Then use a standard ODE solver to solve the obtained system of equations. The merits of this method are (i) having a choice of ODE method separate from spatial discretization, (ii) having higher order of ODE method, and (iii) making use of blackbox ODE solvers with automatic time stepping. This approach is referred to as method of lines (MOL) [2]. MOL is in contrast with full discretization, where both time and spatial domain discretized simultaneously [3].

### 1.3 Finite Element (Conforming)

As mentioned earlier, in MOL the time-dependent PDE is transformed into system of ODEs, then this system of equations can be solved separately from the spatial discretization using an appropriate ODE solver. In this study, we make use of commercial software COMSOL 5.1 to discretize the spatial domain using method of finite element and then solve the obtained system of ODEs with one of the available ODE solvers in COMSOL. More details about different ODE solvers available in COMSOL can be found in [4].

The idea of the FEM is to solve the PDE in a weak sense in contrast to typical form i.e., strong form. Essentially, this method can be summarized in two steps; (i) derivation of weak (variational) form of the problem which has a unique solution in some Sobolev space  $U$ , (ii) finding approximated solution  $u_h$  in some appropriate finite dimensional subspace (conforming)  $U_h$ . By stating the problem in weak form rather than strong one, we can allow more solutions to satisfy the problem i.e., the solutions that satisfy the weak form need less regularity compare to the ones that satisfy the strong form. Consequently, the methods and theories developed for the weak form are more robust. The detailed theory of FEM is available in [5].

## 1.4 Error Analysis

Generally, in solving PDEs, the obtained numerical solution  $u_h$  is experiencing an error in comparison to the true solution  $u$ . This error in the MOL approach for time-dependent PDE's consists of two separate contributions from time discretization (ODE solver) and spatial discretization (FEM). We will refer them to as time-error and spatial-error, respectively through the course of this study. Provided that, the time-error does not dominate the spatial-error, the appropriate norm of this error can be bounded in terms of mesh spacing  $h$  of the discretized spatial domain. Such estimates have the form of  $\|u - u_h\| \leq C h^q$  where  $C$  is a problem-dependent constant independent of  $h$  and the constant  $q$  indicates the order of convergence of the numerical method as the mesh spacing  $h$  decreases [5]. We see from this form of the error estimate that we need  $q > 0$  for convergence as  $h \rightarrow 0$ . More realistically, we wish to have for instance  $q = 1$  for linear convergence,  $q = 2$  for quadratic convergence, or higher values for even faster convergence.

As discussed in great detail in [5],  $\|\cdot\|_\infty$  is not natural norm for FEM. One appropriate norm for FEM errors is the  $L^2(\Omega)$ -norm associated with the space  $L^2(\Omega)$  of square-integrable functions, that is, the space of all functions  $v(x)$  whose square  $v^2(x)$  can be integrated over all  $x \in \Omega$  without the integral becoming infinite. The norm is defined concretely as the square root of that integral, namely

$$\|v\|_{L^2(\Omega)} := \left( \int (v(\mathbf{x}))^2 d\mathbf{x} \right)^{1/2}. \quad (4)$$

Using the  $L^2(\Omega)$ -norm to measure the error of the FEM allows the computation of norms of errors also in cases where the solution and its error do not have derivatives. Lagrange finite elements of degree  $p$ , such as available in COMSOL with  $p = 1, \dots, 5$ , approximate the PDE solution at several points in each element of the mesh such that the restriction of the FEM solution  $u_h$  to each element is a polynomial of degree up to  $p$  in each spatial variable and  $u_h$  is continuous across all boundaries between neighboring mesh elements throughout  $\Omega$ . For the case of linear (degree  $p = 1$ ) Lagrange elements, we have the well known a priori bound (e.g., [5, Section II.7])

$$\|u - u_h\|_{L^2(\Omega)} \leq C h^2, \quad (5)$$

provided  $u \in H^2(\Omega)$ . This assumption on  $u$  is ensured if the right-hand side of the PDE (1) satisfies  $f \in L^2(\Omega)$ . We notice that the convergence order is one higher than the polynomial degree used by the Lagrange elements. Analogously, a more general result for using Lagrange elements with degrees  $p \geq 1$  is that we can expect an error bound of

$$\|u - u_h\|_{L^2(\Omega)} \leq C h^{p+1}, \quad (6)$$

provided  $u \in H^k(\Omega)$  with  $k \geq p + 1$ .

With the above introduction, in the Sec. 2 the time-dependent test problem is stated concretely and solved using FEM with COMSOL 5.1. In Sec. 3 the convergences study is carried out with linear and quadratic Lagrange elements  $p = 1$  and 2 for different ODE solver configurations. Furthermore, in the appendix, the detailed instruction on implementing the convergence study obtained in Sec. 2 is presented using the graphical user interface (GUI) of COMSOL 5.1. The current study is a follow-up to [6, 7], where the FEM convergence studies for two and three dimensional elliptic PDE with smooth and non-smooth source terms were carried out in COMSOL 5.1.

## 2 Parabolic Test Problem

In (1)–(3), the general form of time-dependent parabolic PDE is shown. We consider the classic time-dependent test problem, also known as heat equation, on a polygonal domain, which can be partitioned into the finite element mesh without error. By setting  $D = 1$ ,  $a_0 = 0$ ,  $r = 0$ , and  $u_{ini}(x, y) = 0$  in (1)–(3), and starting at  $t_0 = 0$  we get

$$u_t - \Delta u = f \quad \text{in } \Omega \text{ for } 0 < t \leq t_{fin}, \quad (7)$$

$$\mathbf{n} \cdot \nabla u = 0 \quad \text{on } \partial\Omega \text{ for } 0 < t \leq t_{fin}, \quad (8)$$

$$u = 0 \quad \text{in } \bar{\Omega} \text{ at } t = 0, \quad (9)$$

on two-dimensional domain  $\Omega = (0, 1) \times (0, 1) \subset \mathbb{R}^2$  with the source term  $f$  supplied as

$$\begin{aligned} f(x, y, t) = & (2t/\tau^2)e^{-t^2/\tau^2} \sin^2(\pi x) \sin^2(\pi y) \\ & - 2\pi^2(1 - e^{-t^2/\tau^2}) [\cos(2\pi x) \sin^2(\pi y) + \sin^2(\pi x) \cos(2\pi y)] \end{aligned} \quad (10)$$

This problem has been chosen as it has a known analytical solution

$$u(x, y, t) = (1 - e^{-t^2/\tau^2}) \sin^2(\pi x) \cos^2(\pi y) \quad (11)$$

We use coefficient  $\tau = 2$  and  $t_{fin} = 10$  s for this study. It can be shown that the above problem with the mentioned coefficient tend to steady state,  $u_{ss} = \sin^2(\pi x) \sin^2(\pi y)$ , as  $t \rightarrow \infty$ .

Figs. 1 through 4 show the numerical solution  $u_h$  and its corresponding error ( $u_h - u$ ) for linear and quadratic Lagrange elements with one level of mesh refinement  $m = 1$ . More specifically, Figs. 1 and 2 are obtained using 104 linear Lagrange elements with corresponding degree of freedom DOF = 65 while, Figs. 3 and 4 are obtained using same number of quadratic elements with corresponding degree of freedom DOF = 233. In both cases considered in this study for a degree of Lagrange elements, the obtained solution is consistent with the behavior of the true solution i.e., it gradually grows as  $t$  increases to its steady state which is occurring around  $t \approx 5$  s (see Figs. 1 and 3). Nevertheless, the solution obtained using linear Lagrange elements is not reflecting the smoothness of the true solution stated in (11). As shown in Fig. 1, the flat patches between nodes are clearly recognizable. This shows that for linear Lagrange elements the mesh is not sufficiently fine. On the other hand, Fig. 3 which shows the FEM solution using quadratic Lagrange elements with same level of mesh refinement and same number of elements consequently, shows much smoother results. Also, by comparing the numerical error obtained using linear and quadratic Lagrange elements and plotted in Figs. 2 and 4, respectively we can see that the results obtained using quadratic Lagrange elements are more accurate than the linear ones. The above observations confirm the capability of quadratic elements in producing more accurate and smoother results in compare to linear elements.

## 3 Convergence Study

The problem stated as above is used for observing the convergence of the parabolic test problem. By selecting a test problem which has a known PDE solution  $u$ , the error  $u - u_h$  and its norm in (6) can be directly computed for every desired time in the timespan  $[0, t_{fin}]$ . The convergence order  $q$  is then estimated from these computational results by the following steps: For time  $t_d$ , starting from some initial mesh, we refine it regularly repeatedly, which subdivides every triangle of the two-dimensional mesh uniformly into four congruent triangles. If  $h$  measures the maximum side length of all triangles, this procedure halves the value of  $h$  in each refinement. Let  $m$  denote the number of refinement levels from the initial mesh and  $E_m := \|u - u_h\|_{L^2(\Omega)}$  the error norm on that level. Then assuming that  $E_m = C h^q$ , the error for the next coarser mesh with mesh spacing  $2h$  is  $E_{m-1} = C (2h)^q = 2^q C h^q$ . Their ratio is then  $R_m = E_{m-1}/E_m = 2^q$  and  $Q_m = \log_2(R_m)$  provides us with a computable estimate for  $q$  in (6) as  $h \rightarrow 0$ . Notice that the technique described here uses the known PDE solution  $u$ ; this is in contrast to the technique described in [8] that worked for Lagrange elements with  $p = 1$  without knowing the PDE solution  $u$ .

Tables 1 and 2 show the convergence study for linear ( $p = 1$ ) and quadratic ( $p = 2$ ) Lagrange elements, respectively. In both tables, the number of elements  $N_e$ , the number of vertices  $N_v$ , the number degrees of

freedom (DOF), the FEM error  $E_m = \|u - u_h\|_{L^2(\Omega)}$ , the ratio of errors of consecutive refinements  $R_m = E_{m-1}/E_m$ , and the estimate  $Q_m = \log_2(R_m)$  for the convergence order for each refinement level  $m$  at  $t = 1, 2, 3, 4, 5$  and  $10$  s are tabulated. Also, the results in aforementioned tables are obtained using COMSOL default values of relative and absolute tolerances in time-dependent solver. In COMSOL 5.1 these values are `RelTol = 0.01` and `AbsTol = 0.001`, respectively.

The column DOF lists the numbers of degrees of freedom, which is the number of unknowns for the finite element method that need to be solved for, in the system of linear equations and thus determine the computational complexity of the problem. For linear Lagrange elements ( $p = 1$ ) with the unknowns at the vertices of the mesh, the DOF are equal to  $N_v$ . For higher order Lagrange elements, additional degrees of freedom are unknowns in each element, which increases the accuracy of the solution compared to lower order Lagrange elements on meshes with the same number of elements. This is born out by the FEM errors in the column  $E_m$ , which get smaller not just with refinement level within each sub-table, but are also smaller as  $p$  increases from one sub-table to the next for corresponding refinement levels and their meshes. In fact, comparing not corresponding refinement levels and their meshes, but comparing (approximately) equal DOF from one sub-table to the next ones, we see that higher order Lagrange elements result in smaller errors, for identical complexity of the linear system solve.

As shown in Tables 1, the convergence order for linear Lagrange elements  $p = 1$ , is almost  $q \approx 2$  for first two refinement levels  $m = 1, 2$  then it decrease dramatically as level refinement  $m$  increases. This behavior holds true for all times  $t = 1, 2, 3, 4, 5$ , and  $10$  s. This clearly contradicts the FEM theory which predicts convergence order of  $q = 2$  for linear Lagrange elements. For the quadratic Lagrange elements case ( $p = 2$ ), as shown in Table 2 things get worse. The expected convergence order cannot be observed even for the first refinement levels.

The reason of this behavior is the fact that with default values of absolute and relative tolerances, the time-error (the error due to ODE solver) dominates the spatial error. And as a result the true convergence order of FEM due to spatial refinement cannot be observed. By decreasing aforementioned tolerances in COMSOL we can overcome this problem. It turns out that, with linear Lagrange elements  $p = 1$  setting relative and absolute tolerances to `RelTol=1e-5`, and `AbsTol=1e-8`, respectively make the spatial-error, dominant for 4 levels of mesh refinement. The results with these new configurations are tabulated in Table 3.

For quadratic Lagrange elements  $p = 2$  we even need lower values of tolerances to be able to observe the convergence order of FEM for this problem. The new values are set to `1e-8` for relative tolerance and `1e-10` for absolute tolerance. The new results are tabulated in Table 4.

As expected for a convergent method, we can observe qualitatively that the errors  $E_m$  for all times in sub-tables of Tables 3 and 4 tend to zero as the number of refinements increases and thus the mesh size  $h$  tends to zero. Quantitatively, the quantities  $R_m$  and  $Q_m$  tend to constant values in each sub-table. This means that the errors decrease systematically with each smaller mesh size, namely  $Q_m$  tends to  $p + 1$  in each table, which confirms the order of convergence  $q = p + 1$  in (6) for both  $p = 1$  and  $2$  presented in this study. These results demonstrate the advantage of using higher-order finite elements, if the regularity of the problem allows them.

## 4 Conclusions

In this study, the time-dependent PDE test problem i.e., the heat equation has been solved by a MOL approach using FEM with the commercial FEM software COMSOL 5.1. The convergence study was carried out for Lagrange elements of degree  $p = 1$  and  $p = 2$ . It has been shown that for both cases considered in this study, the COMSOL default relative and absolute tolerances are not sufficiently low to make the spatial-error dominant. Consequently, the observed convergence ratios with default values of tolerances were not consistent with theory. We were able to capture the correct convergence ratios by modifying relative and absolute tolerances in COMSOL time-dependent solver. Moreover we confirmed that, for the time-dependent test problem considered in this study, the convergence order of FEM using quadratic Lagrange elements is greater than the linear ones.

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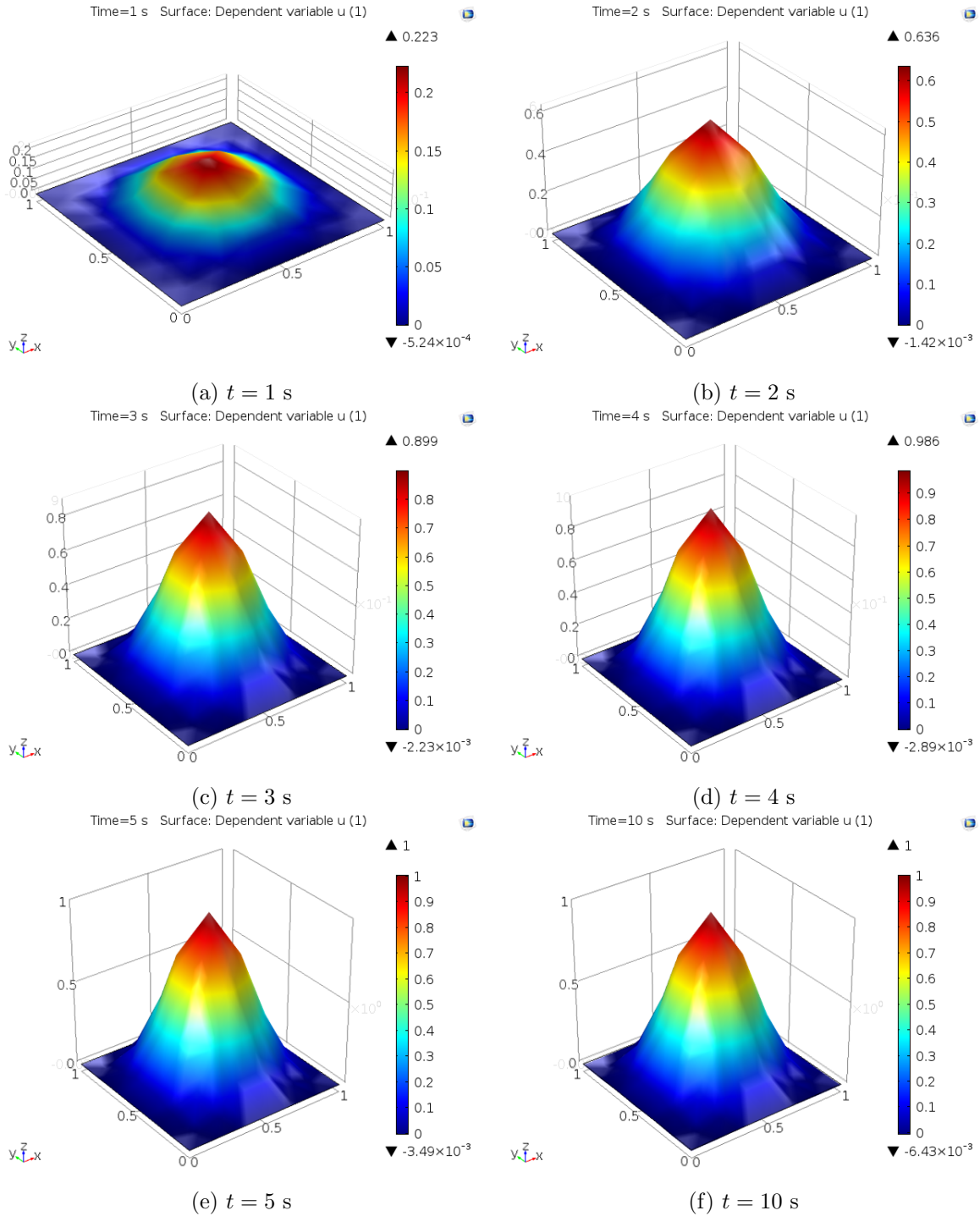


Figure 1: The numerical solution  $u_h$  for time-dependent test problem (7)–(9). The results are obtained using *linear* Lagrange elements on a mesh with 104 mesh elements. The degree of freedom solved for is  $\text{DOF} = 65$ . The results are reported at 6 different times as indicated.

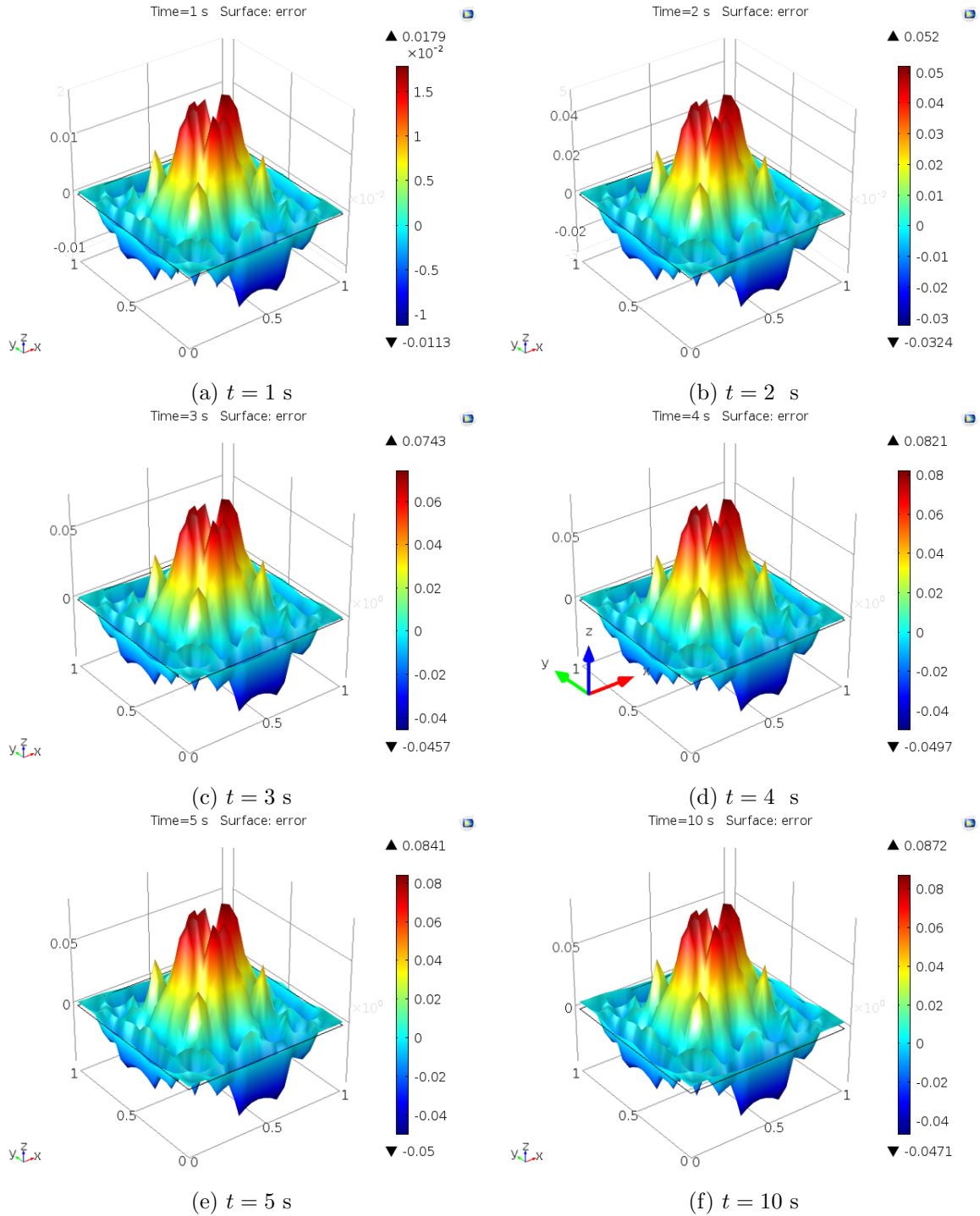


Figure 2: The numerical error ( $u_h - u$ ) for time-dependent test problem (7)–(9). The results are obtained using *linear* Lagrange elements on a mesh with 104 mesh elements. The degree of freedom solved for is  $\text{DOF} = 65$ . The results are reported at 6 different times as indicated.

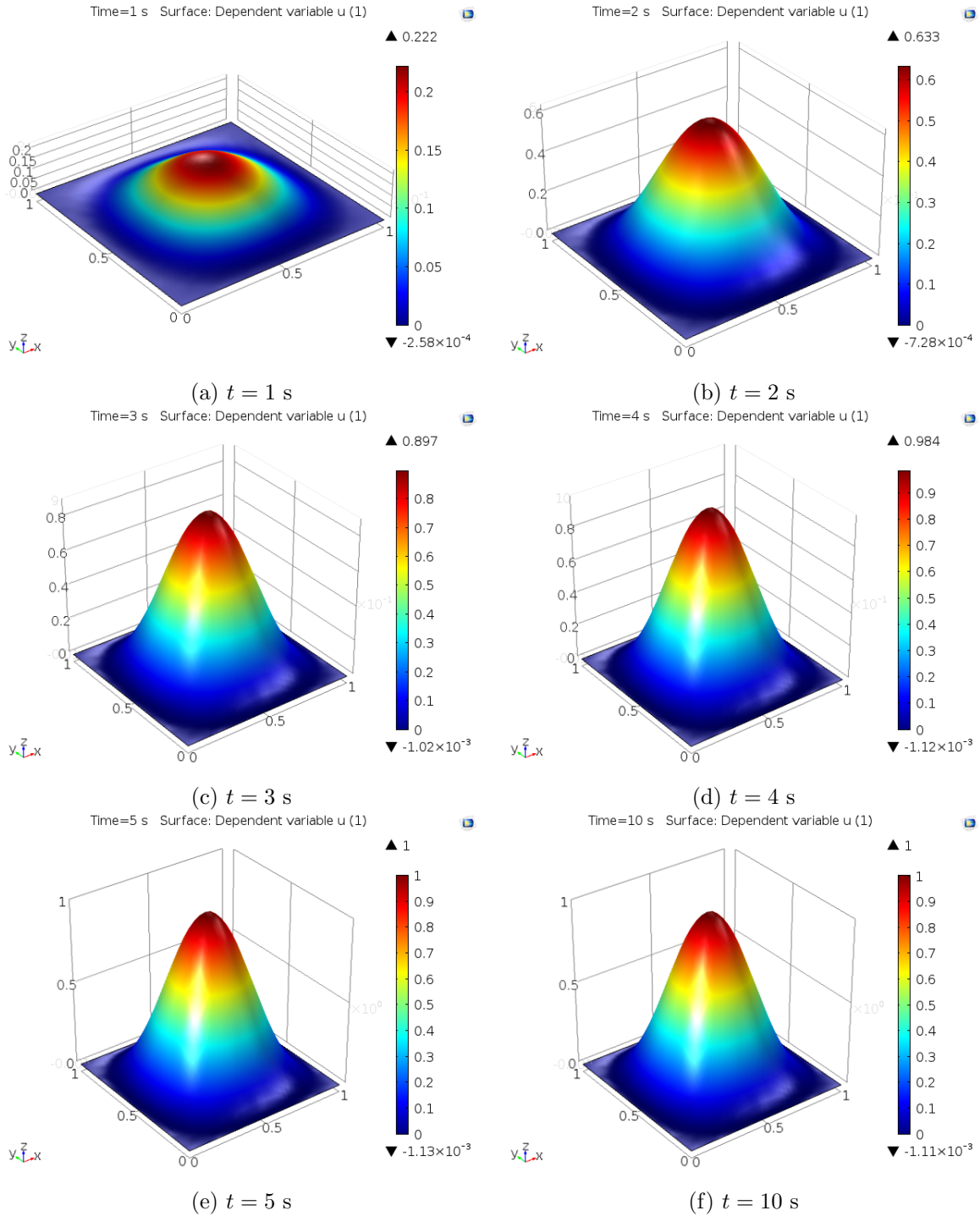


Figure 3: The numerical solution  $u_h$  for time-dependent test problem (7)–(9). The results are obtained using *linear* Lagrange elements on a mesh with 104 mesh elements. The degree of freedom solved for is  $\text{DOF} = 233$ . The results are reported at 6 different times as indicated.



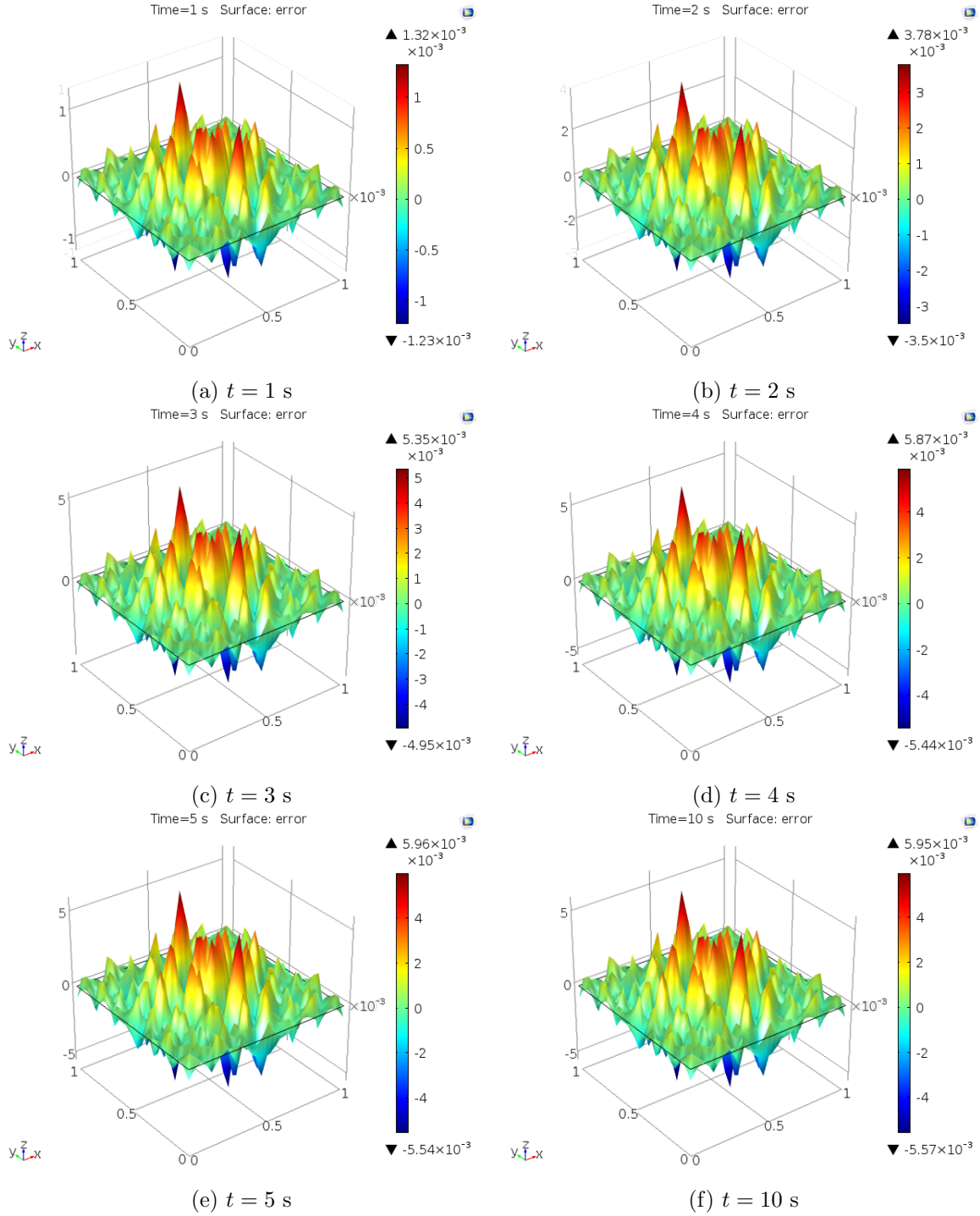


Figure 4: The numerical error ( $u_h - u$ ) for time-dependent test problem (7)–(9). The results are obtained using *linear* Lagrange elements on a mesh with 104 mesh elements. The degree of freedom solved for is  $\text{DOF} = 233$ . The results are reported at 6 different times as indicated.

Table 1: Convergence study for the time-dependent test problem (7)–(9) using linear Lagrange elements  $p = 1$  for time  $t = 1, 2, 3, 4, 5$  and 10 s as indicated in each sub-table. For each  $t$ , the refinement level  $m$ , the number of elements  $N_e$  in the mesh, the number of vertices  $N_v$ , the number of degrees of freedom (DOF), the FEM error  $E_m = \|u - u_h\|_{L^2(\Omega)}$ , the ratio of errors of consecutive refinements  $R_m = E_{m-1}/E_m$ , and the estimate  $Q_m = \log_2(R_m)$  for the convergence order is tabulated. The results are obtained using default values of absolute and relative ODE tolerances in COMSOL 5.1 (0.001, and 0.01, respectively).

	$m$	$N_e$	$N_v$	$DOF$	$E_m$	$R_m$	$Q_m$
$t = 1$ s	0	26	20	20	2.322E-02	NA	NA
	1	104	65	65	5.716E-03	4.06	2.02
	2	416	233	233	1.525E-03	3.75	1.91
	3	1,664	881	881	5.940E-04	2.57	1.36
	4	6,656	3,425	3,425	4.688E-04	1.27	0.34
$t = 2$ s	0	26	20	20	6.710E-02	NA	NA
	1	104	65	65	1.641E-02	4.09	2.03
	2	416	233	233	4.027E-03	4.08	2.03
	3	1,664	881	881	9.452E-04	4.26	2.09
	4	6,656	3,425	3,425	3.438E-04	2.75	1.46
$t = 3$ s	0	26	20	20	9.651E-02		
	1	104	65	65	2.344E-02	4.12	2.04
	2	416	233	233	5.938E-03	3.95	1.98
	3	1,664	881	881	1.613E-03	3.68	1.88
	4	6,656	3,425	3,425	7.932E-04	2.03	1.02
$t = 4$ s	0	26	20	20	1.086E-01	NA	NA
	1	104	65	65	2.557E-02	4.25	2.09
	2	416	233	233	6.413E-03	3.99	2.00
	3	1,664	881	881	1.919E-03	3.34	1.74
	4	6,656	3,425	3,425	1.334E-03	1.44	0.52
$t = 5$ s	0	26	20	20	1.151E-01	NA	NA
	1	104	65	65	2.629E-02	4.38	2.13
	2	416	233	233	7.418E-03	3.54	1.83
	3	1,664	881	881	3.779E-03	1.96	0.97
	4	6,656	3,425	3,425	3.415E-03	1.11	0.15
$t = 10$ s	0	26	20	20	1.559E-01	NA	NA
	1	104	65	65	2.628E-02	5.93	2.57
	2	416	233	233	7.795E-03	3.37	1.75
	3	1,664	881	881	4.618E-03	1.69	0.76
	4	6,656	3,425	3,425	4.334E-03	1.07	0.09

Table 2: Convergence study for the time-dependent test problem (7)–(9) using quadratic Lagrange elements  $p = 2$  for time  $t = 1, 2, 3, 4, 5$  and 10 s as indicated in each sub-table. For each  $t$ , the refinement level  $m$ , the number of elements  $N_e$  in the mesh, the number of vertices  $N_v$ , the number of degrees of freedom (DOF), the FEM error  $E_m = \|u - u_h\|_{L^2(\Omega)}$ , the ratio of errors of consecutive refinements  $R_m = E_{m-1}/E_m$ , and the estimate  $Q_m = \log_2(R_m)$  for the convergence order is tabulated. The results are obtained using default values of absolute and relative ODE tolerances in COMSOL 5.1 (0.001, and 0.01, respectively).

	$m$	$N_e$	$N_v$	$DOF$	$E_m$	$R_m$	$Q_m$
$t = 1$ s	0	26	20	65	1.434E-03	NA	NA
	1	104	65	233	5.186E-04	2.76	1.47
	2	416	233	881	4.570E-04	1.13	0.18
	3	1,664	881	3,425	4.557E-04	1.00	0.00
	4	6,656	3,425	13,505	4.557E-04	1.00	0.00
$t = 2$ s	0	26	20	65	3.872E-03	NA	NA
	1	104	65	233	7.473E-04	5.18	2.37
	2	416	233	881	3.719E-04	2.01	1.01
	3	1,664	881	3,425	3.662E-04	1.02	0.02
	4	6,656	3,425	13,505	3.663E-04	1.00	0.00
$t = 3$ s	0	26	20	65	5.522E-03	NA	NA
	1	104	65	233	1.210E-03	4.56	2.19
	2	416	233	881	7.366E-04	1.64	0.72
	3	1,664	881	3,425	7.268E-04	1.01	0.02
	4	6,656	3,425	13,505	7.267E-04	1.00	0.00
$t = 4$ s	0	26	20	65	6.535E-03	NA	NA
	1	104	65	233	1.698E-03	3.85	1.94
	2	416	233	881	1.351E-03	1.26	0.33
	3	1,664	881	3,425	1.347E-03	1.00	0.00
	4	6,656	3,425	13,505	1.347E-03	1.00	0.00
$t = 5$ s	0	26	20	65	8.099E-03	NA	NA
	1	104	65	233	3.594E-03	2.25	1.17
	2	416	233	881	3.397E-03	1.06	0.08
	3	1,664	881	3,425	3.388E-03	1.00	0.00
	4	6,656	3,425	13,505	3.385E-03	1.00	0.00
$t = 10$ s	0	26	20	65	1.058E-02	NA	NA
	1	104	65	233	4.518E-03	2.34	1.23
	2	416	233	881	4.325E-03	1.04	0.06
	3	1,664	881	3,425	4.315E-03	1.00	0.00
	4	6,656	3,425	13,505	4.311E-03	1.00	0.00

Table 3: Convergence study for the time-dependent test problem (7)–(9) using linear Lagrange elements  $p = 1$  for time  $t = 1, 2, 3, 4, 5$  and 10 s as indicated in each sub-table. For each  $t$ , the refinement level  $m$ , the number of elements  $N_e$  in the mesh, the number of vertices  $N_v$ , the number of degrees of freedom (DOF), the FEM error  $E_m = \|u - u_h\|_{L^2(\Omega)}$ , the ratio of errors of consecutive refinements  $R_m = E_{m-1}/E_m$ , and the estimate  $Q_m = \log_2(R_m)$  for the convergence order is tabulated. The results are obtained with relative and absolute ODE tolerances being  $10^{-5}$  and  $10^{-8}$ , respectively.

	$m$	$N_e$	$N_v$	$DOF$	$E_m$	$R_m$	$Q_m$
$t = 1$ s	0	26	20	20	2.318E-02	NA	NA
	1	104	65	65	5.676E-03	4.08	2.03
	2	416	233	233	1.433E-03	3.96	1.99
	3	1,664	881	881	3.596E-04	3.99	2.00
	4	6,656	3,425	3,425	8.997E-05	4.00	2.00
$t = 2$ s	0	26	20	20	6.712E-02	NA	NA
	1	104	65	65	1.648E-02	4.07	2.03
	2	416	233	233	4.170E-03	3.95	1.98
	3	1,664	881	881	1.046E-03	3.98	1.99
	4	6,656	3,425	3,425	2.619E-04	4.00	2.00
$t = 3$ s	0	26	20	20	9.644E-02	NA	NA
	1	104	65	65	2.346E-02	4.11	2.04
	2	416	233	233	5.938E-03	3.95	1.98
	3	1,664	881	881	1.490E-03	3.98	1.99
	4	6,656	3,425	3,425	3.730E-04	4.00	2.00
$t = 4$ s	0	26	20	20	1.087E-01	NA	NA
	1	104	65	65	2.582E-02	4.21	2.07
	2	416	233	233	6.530E-03	3.95	1.98
	3	1,664	881	881	1.639E-03	3.98	1.99
	4	6,656	3,425	3,425	4.103E-04	4.00	2.00
$t = 5$ s	0	26	20	20	1.150E-01	NA	NA
	1	104	65	65	2.630E-02	4.37	2.13
	2	416	233	233	6.643E-03	3.96	1.98
	3	1,664	881	881	1.667E-03	3.98	1.99
	4	6,656	3,425	3,425	4.173E-04	4.00	2.00
$t = 10$ s	0	26	20	20	1.561E-01	NA	NA
	1	104	65	65	2.672E-02	5.84	2.55
	2	416	233	233	6.661E-03	4.01	2.00
	3	1,664	881	881	1.671E-03	3.99	2.00
	4	6,656	3,425	3,425	4.182E-04	4.00	2.00

Table 4: Convergence study for the time-dependent test problem (7)–(9) using quadratic Lagrange elements  $p = 2$  for time  $t = 1, 2, 3, 4, 5$  and 10 s as indicated in each sub-table. For each  $t$ , the refinement level  $m$ , the number of elements  $N_e$  in the mesh, the number of vertices  $N_v$ , the number of degrees of freedom (DOF), the FEM error  $E_m = \|u - u_h\|_{L^2(\Omega)}$ , the ratio of errors of consecutive refinements  $R_m = E_{m-1}/E_m$ , and the estimate  $Q_m = \log_2(R_m)$  for the convergence order is tabulated. The results are obtained with relative and absolute ODE tolerances being  $10^{-8}$  and  $10^{-10}$ , respectively.

	$m$	$N_e$	$N_v$	$DOF$	$E_m$	$R_m$	$Q_m$
$t = 1$ s	0	26	20	65	1.362E-03	NA	NA
	1	104	65	233	2.433E-04	5.60	2.49
	2	416	233	881	3.153E-05	7.71	2.95
	3	1,664	881	3,425	3.980E-06	7.92	2.99
	4	6,656	3,425	13,505	4.993E-07	7.97	2.99
$t = 2$ s	0	26	20	65	3.918E-03	NA	NA
	1	104	65	233	6.964E-04	5.63	2.49
	2	416	233	881	9.016E-05	7.72	2.95
	3	1,664	881	3,425	1.138E-05	7.93	2.99
	4	6,656	3,425	13,505	1.427E-06	7.97	3.00
$t = 3$ s	0	26	20	65	5.578E-03	NA	NA
	1	104	65	233	9.862E-04	5.66	2.50
	2	416	233	881	1.276E-04	7.73	2.95
	3	1,664	881	3,425	1.610E-05	7.93	2.99
	4	6,656	3,425	13,505	2.019E-06	7.97	3.00
$t = 4$ s	0	26	20	65	6.181E-03	NA	NA
	1	104	65	233	1.082E-03	5.71	2.51
	2	416	233	881	1.401E-04	7.73	2.95
	3	1,664	881	3,425	1.767E-05	7.93	2.99
	4	6,656	3,425	13,505	2.216E-06	7.97	3.00
$t = 5$ s	0	26	20	65	6.381E-03	NA	NA
	1	104	65	233	1.101E-03	5.80	2.54
	2	416	233	881	1.424E-04	7.73	2.95
	3	1,664	881	3,425	1.796E-05	7.93	2.99
	4	6,656	3,425	13,505	2.253E-06	7.97	3.00
$t = 10$ s	0	26	20	65	7.356E-03	NA	NA
	1	104	65	233	1.104E-03	6.67	2.74
	2	416	233	881	1.427E-04	7.74	2.95
	3	1,664	881	3,425	1.800E-05	7.93	2.99
	4	6,656	3,425	13,505	2.257E-06	7.97	3.00

# A COMSOL: Using the Graphical User Interface (GUI)

## A.1 Setup and Solution

1. Once the GUI loads, choose Model Wizard, then choose 2D on the Select a Space Dimension page. The Model Wizard will take you automatically to the Select Physics page.
2. On the Select Physics page, expand the Mathematics branch (by clicking on the arrow to the left of the label) and then the PDE Interfaces branch, and select the Coefficient Form PDE node. Click the Add button. By default, the number of dependent variables is one and the variable name is  $u$ . Since this is the desired setup for the problem, click the Study button (right arrow).
3. Under the Select Study page, select Time Dependent and click the Done button (checkered flag) on the bottom of this page.
4. Before proceeding to establish the specifics of the test problem, check to ensure that all needed information will easily be displayed. In the Model Builder window in the left pane of the GUI, click the Show Menu (eye with a bar symbol) on the toolbar and make sure that Discretization is checked; this is needed to enable user to change element order as will be discussed in step 10 below. This setting is saved from one COMSOL session to the next, so once this is selected, COMSOL will retain this selection for future restarts.
5. In COMSOL you can define parameters of the problem as a global definition. Defining the parameters in this way has several advantages, like enabling us to do parametric study on them if needed or change them readily. We want to define coefficient  $\tau$  and  $t_f = 10$  s in (7)–(9) as a parameter in COMSOL. To do so, in the Model Builder right click the Global Definitions branch and click Parameters. In the Settings window, under the Parameters section, type **tau** under the Name column in the Parameters table then in the Expression column type  $2[\text{s}]$ . Here,  $[\text{s}]$  is dimension of the parameter **tau**. Now, in the Value column, the cell in front of **tau** should read  $2 \text{ s}$ . Do the same thing for  $t_f = 10$  s.
6. In order to set up the desired domain, right click **Geometry 1** and select Square in the Model Builder window. By default, this will generate the desired square domain  $\Omega = (0, 1) \times (0, 1)$  with one corner of the square at the origin. Select **Build All** under **Geometry 1** to update the geometry.
7. In the Model Builder window in the left window pane, the right-hand side of the PDE can be set by expanding the PDE branch and selecting the **Coefficient Form PDE 1** node. The center pane of the GUI specifies the general form of the equation currently selected as

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla \cdot (-c \nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + a u = f.$$

Under Source Term, enter for  $f$  the expression

$(2*t/\text{tau}^2)*\exp(-t^2/\text{tau}^2)*\sin(\text{pi}*x)^2*\sin(\text{pi}*y)^2-2*\text{pi}^2*(1-\exp(-t^2/\text{tau}^2))*(\cos(2*\text{pi}*x)*\sin(\text{pi}*y)^2+\sin(\text{pi}*x)^2*\cos(2*\text{pi}*y))$ . Leave the other coefficients as their default values in order to establish the heat equation of (7)–(9).

8. By clicking the **Zero Flux 1** node under the Coefficient Form PDE branch, You can see that the desired Neumann boundary condition in (7)–(9) is automatically generated.
9. Also, by clicking **Initial Values 1** node under the Coefficient Form PDE branch, you can see initial value of  $u$  is set to 0 which is desired value for (7)–(9).
10. Again in the Model Builder window in the left pane, select the PDE branch and on the PDE page in the center pane under Discretization (you might have to expand Discretization first), choose Linear for the Element order. This establishes the degree of the Lagrange elements used. By selecting the element order to be Linear, COMSOL will use linear Lagrange elements in the finite element solution.

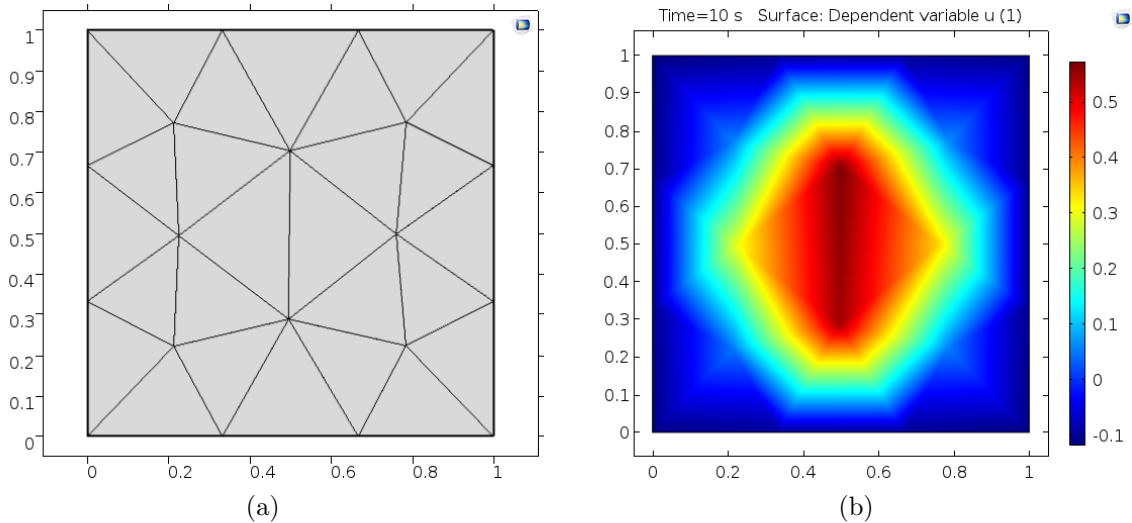


Figure 5: (a) Extremely coarse mesh generated in COMSOL 5.1, (b) two-dimensional view of the FEM solution for heat equation (7)–(9) with linear Lagrange elements ( $p = 1$ ) and 0 level of mesh refinement ( $m = 0$ ) at  $t = 10$  s.

11. In order to generate the FEM mesh that will be used to compute the FEM solution, first right click the **Mesh 1** branch under the Model Builder window and select **Free Triangular** to establish the mesh. On the Free Triangular Settings page in the center pane, under the Domains item, select for Geometric entity level the selection Domain. Under the **Mesh 1** branch, select the **Size** node and on the Size page under Element Size, choose **Extremely coarse** for the Predefined Elements Size. In order to see the mesh being used, right click the **Mesh 1** branch and choose Build All. Fig. 5 (a) displays the extremely coarse mesh that will be used to compute the FEM solution. The number of triangular elements used in this mesh can be determined by right clicking the **Mesh 1** branch and choosing **Statistics**. For this domain and extremely coarse mesh, the number of triangular elements is 26.
12. In a time dependent problem like this one, we have to provide COMSOL with time range that we wish the the software solve the problem for us. This time range has nothing to do with time steps that software choose to solve the ODE obtained by method of lines as discussed earlier. To set the time range, in the Model Builder, expand **Study 1** branch, and click **Step1: Time Dependent**. In the Time Dependent Settings window, in the Study Settings section, locate **Times** and type `range(0,1,t_fin)` to compute the solution at  $t = 1, 2, \dots, 10$  s. Alternatively, you could have clicked the Range button in front of Times section and set the range there.
13. Now, compute the FEM solution by right clicking the **Study 1** branch under the Model Builder window and selecting Compute. Alternatively, one can click the blue equal symbol above the Study page on the toolbar. Once the solution is computed, the degrees of freedom which have been solved for can be seen below the Graphics window in the Messages tab, which is 20 for this coarse mesh using linear Lagrange (element order 1) elements.
14. As discussed in Sec. 1.4, for time dependent problems the error consists of the spatial-error and time-error. And for us to be able to see the convergence order of FEM we need to make sure that relative and absolute tolerances of the ODE solver are sufficiently small that the time-error is not dominant. To change the relative tolerance in COMSOL, under the Study 1 branch, click on **Step1: Time Dependent**, in the Settings window for Step1: Time Dependent click to check mark the **Relative tolerance** and then type the desired value for relative tolerance.

To change the absolute tolerance, expand **Solver Configurations** node under the Study 1 branch then click **Time-Dependent** node in the Setting window for Time Dependent, expand Absolute Tolerance

section, then type the new value of absolute tolerance.

## A.2 Post-Processing

The default plot of the solution is generated at time  $t = 0$ . To see the solution at other time, say 10 s, expand the Results branch in the Model Builder and select **2D Plot Group 1**. In the Settings window for **2D Plot Group 1** under the Data section locate the **Time (s)** and choose 10. The 2-dimensional form of the solution at  $t = 10$  s is shown in Fig. 5 (b). A more conventional way might be to present the solution in a three-dimensional view, as shown in Figs. 1 and 2. This section gives instructions on how to post-process the FEM solution obtained in the previous section by changing the plot to a three-dimensional view and by computing the FEM error.

1. Under the Results branch of the Model Builder window, expand the **2D Plot Group 1** branch, right click on the **Surface 1** node and choose the Height Expression. This shows a three-dimensional surface and height plot of the FEM solution  $u_h(x, y)$  at  $t = 10$  s. The result for one level of mesh refinement  $m = 1$  is shown in Fig. 1 (f). The previous section specifically used linear ( $p = 1$ ) Lagrange elements to solve the problem, which means that the FEM solution  $u_h(x, y)$  is a flat patch on each triangle of the mesh. This is clearly visible in Fig. 1 (f).

Furthermore, in order to control the height of the z-axis, we fixed the scale factor of height expression to be 1 for all the times as indicated in Fig. 1. This can be done by clicking the **Height Expression 1** node under the **2D Plot Group 1** branch. Then in the Height Expression Settings window expand the **Axis** menu. Make sure that the scale factor is check marked. Change its corresponding value to 1.5.

2. In order to construct a plot of the FEM error  $u_h - u$ , right click the **Results** branch and choose **2D Plot Group**. This creates a second plot group called **2D Plot Group 2**. Right Click the **2D Plot Group 2** and select **Surface**. This creates the node **Surface 1** under the **2D Plot Group 2** branch. Select this **Surface 1** node and on the Surface page under expression, type the formula for the error which is the difference between the PDE solution and the FEM solution:

$$(1-\exp(-t^2/\tau^2))*\sin(\pi*x)^2*\sin(\pi*y)^2-u.$$

Then right click this **Surface 1** node and select the Height Expression. Fig. 2 shows a three-dimensional surface and height plot of the error at 6 different times as indicated for one level of mesh refinement  $m = 1$ .

3. The convergence studies of the FEM solution rely on the  $L^2(\Omega)$ -norm  $E_m = \|u - u_h\|_{L^2(\Omega)}$  of the FEM error with the norm defined in (4) with  $v = u - u_h$ . COMSOL can compute this norm. There are two ways to compute it in COMSOL. While first method compute the norm  $E_m$  directly, second method compute the integral  $\int (u - u_h)^2 dx$  that appears in the norm definition which is then the square  $E_m^2$  of the desired norm  $E_m$ .

**Method 1** One way to compute the  $L^2(\Omega)$ -norm, is to add a component coupling operator to compute a derived global quantity from the model. These operators can be convenient for results processing and COMSOL's solvers can also use them during the solution process. As already mentioned, the advantage of this method is that, in this way we can directly compute the  $L^2(\Omega)$ -norm rather than its square. To do so, right click **Definitions** under the **Component 1 Branch** go to the **Component Coupling** and choose **Integration**, in the **Source Selection** section in the Settings window for **Integration** choose **All domain** for **Selection**. Note that the default name for this operator is **intop1**. From now on, this operator can be used for integrating the desired quantities over the domain. In order to be able to use this operator in post processing you need to recompute the solution.

After recomputing the FEM solution, right click **Derived Values** under the **Results** branch and choose **Global Evaluation**. Select **Global Evaluation 1** node, in the setting window, and under **Expression** section type **sqrt(intop1((sin(pi\*x)^2\*sin(pi\*y)^2-u)^2))**. Click to check mark the **Description** and label this quantity by typing  $E_m$  to indicate that it is the the norm of the error. Now, right click the **Global Evaluation 1** node on the **Model Builder** window and select



Evaluate and New Table. This will compute the norm  $E_m$  for all times i.e.,  $t = 1, 2, \dots, 10$  s. The result of the computation shown in the Table 1 tab under the graphics area.

**Method 2** Right click the **Derived Values** node under the Results branch on the Model Builder and select Surface Integration. Choose the desired time that you want to calculate the error at ( $t = 10$  s in this case). Choose all domains under Selection on the Surface Integration Page. Below the Expression section, type the square  $(u - u_h)^2$  of the error as  $((1 - \exp(-t^2/\tau^2)) * \sin(\pi * x)^2 * \sin(\pi * y)^2 - u)^2$ .

Click to check mark the Description and label this quantity by typing  $E_m^2$  to indicate that it is the square of the norm of the error. Now, right click the **Surface Integration** node on the Model Builder window and select Evaluate and New Table. The result of the computation is shown in the Table 2 tab under the graphics area.

4. It is useful to save the solution process as a COMSOL mph-file at this stage before mesh refinements to have it available as starting point later when considering higher order Lagrange elements. Under the **File** menu, choose **Save As ...**. For reference, we will name the file `heat_equation_2d`. This will automatically save as an mph file and append the extension `mph` to the chosen filename. This file `heat_equation_2d` is posted along with this tech. report at the webpage `hpcf.umbc.edu` under Publications.

### A.3 Convergence Studies

In this section, we make use of the steps discussed in App. A.2 in order to carry out a convergence study. We repeatedly refine the mesh that was used to compute the FEM solution, recompute the solution and its error norm, and then copy all calculated error norms.

1. Refine the mesh by right clicking the **Mesh 1** branch and under More Operations select Refine. In the Refine Settings window under Refine Options, type 1 for Number of refinements and rebuild the mesh by right clicking the **Mesh 1** branch and selecting Build All. Again, check the statistics by right clicking the **Mesh 1** branch and selecting **Statistics**. With one refinement, the number of triangular nodes has increased by a factor of 4 to a total of 104 elements.
2. Recompute the FEM solution under this refinement by right clicking the **Study 1** branch and selecting Compute. Here you can solve the problem only for  $t = 0, 1, 2, 3, 4, 5$  and 10 s rather than the whole range of  $1, 2, \dots, 10$  s; just change the `range(0,1,t_fin)` to `range(0,1,5),t_fin`. Once the solution is computed, either right click the **Surface Integration 1** or **Global Evaluation 1** node and select Evaluate and choose **Table 1** (or **Table 2**) to add the result to the previously created tables (make sure that you evaluate error for all desired times). Continue this process through several refinements. Depending on the method that you have used for calculating the error, the Table tab under the graphics window accumulates all results for  $E_m^2$  or  $E_m$  over the course of these refinements.
3. After following the above procedure through 4 consecutive refinements, we can copy the data for the  $E_m$  of the FEM errors from the table under the Results tab into some other software, such as MATLAB, for further processing. The remaining columns in Tables 1 through 4 can be readily computed by using the formulas  $R_m = E_{m-1}/E_m$  and  $Q_m = \log_2(R_m)$ .

Following the previous steps in this section provides a convergence study for the Lagrange elements of order  $p = 1$  with default relative and absolute tolerances, `RelTol=0.01` and `AbsTol=0.001`. In order to perform convergence studies for higher order Lagrange elements and/or different tolerances, start from the mph-file from the end of App. A.2 that was saved before any mesh refinements. From the **File** menu, choose **Open** to load the file. Once the file is loaded, follow the procedure described in step 10 and 14 in App. A.1 to change the element order  $p$  and tolerances, respectively.