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Finite Element Convergence for Time-Dependent PDEs with a Point Source in COMSOL 4.2

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Abstract: The FEM theory provides the basis for quantification on the accuracy and reliability of a numerical solution by the a priori error estimates on the FEM error vs. the mesh spacing of the FEM mesh. This paper presents information on the techniques needed in COMSOL 4.2 to enable computational studies that demonstrate this theory for time-dependent problems, in extension of previous work on stationary problems. These techniques can be used in many general settings, including when the analytic PDE solution is not known.

We consider the time-dependent linear heat equation with homogeneous Dirichlet boundary conditions in both two and three spatial dimensions with both a smooth source term and a non-smooth point source term modeled by one Dirac delta function located at the center of the domain. The presence of the point source for all positive times results in a problem for which no analytic solution is known. The observed constant slope for errors at several representative times in conventional log-log plots of the FEM error versus the reciprocal of the mesh size confirms the exponent of the mesh size in the error estimate to agree with recent theory for the problem.

This paper presents information on the techniques needed in COMSOL 4.2 to enable the studies, including how to correctly implement the Dirac delta function for a time-dependent problem, how to set up a study with repeated uniform mesh refinement at several points in time as needed for a time-dependent PDE problem, how to use a reference solution since no analytic PDE solution is known, how to collect data from each refinement level and compute the convergence order from them, and more.

Key words: Heat equation, a priori error estimate, convergence study, mesh refinement.

1 Introduction

The finite element method (FEM) is a powerful numerical method for solving partial differential equations (PDEs), such as for instance the time-dependent linear parabolic heat equation with homogeneous Dirichlet boundary conditions

$$u_t - \nabla \cdot \nabla u = f \quad \text{for } x \in \Omega \text{ and } 0 < t \le T, \tag{1.1}$$

$$u = 0 \quad \text{for } x \in \partial\Omega \text{ and } 0 < t \le T, \tag{1.2}$$

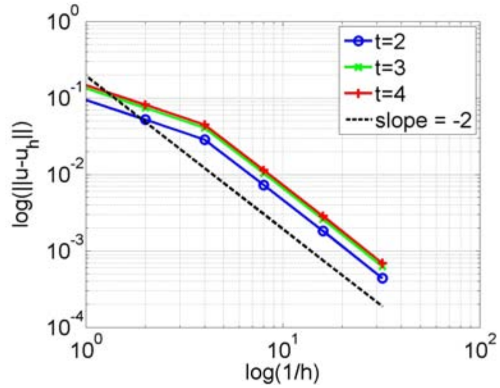
$$u = 0 \quad \text{for } x \in \overline{\Omega} \text{ at } t = 0, \tag{1.3}$$

where f is a given source term on the domain $\Omega \subset \mathbb{R}^d$ in $d = 2$ and 3 dimensions. We consider the simple domain $\Omega = (-1, 1)^d$ and the initial condition $u = 0$ for compatibility with the boundary conditions in order to focus the numerical studies on the properties of the source term f.

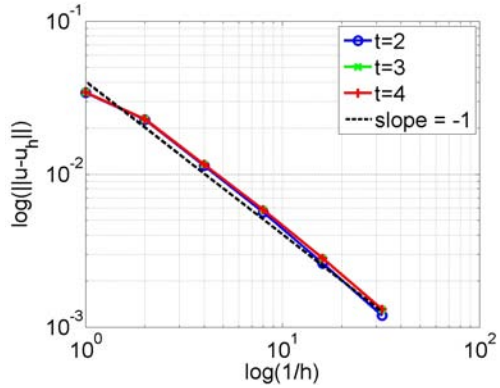
The FEM theory provides the basis for quantification on the accuracy and reliability of a numerical solution by the a priori error estimate

$$\|u(\cdot, t) - u_h(\cdot, t)\|_{L^2(\Omega)} \le C\, h^{\lambda}, \tag{1.4}$$

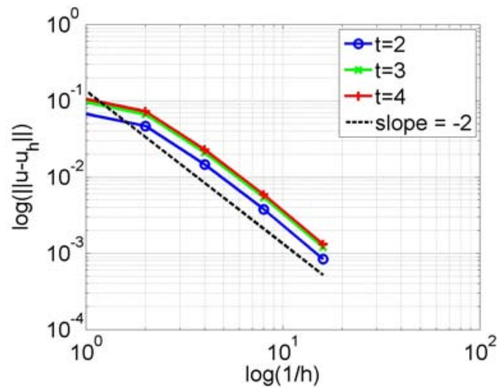
as $h \to 0$, for all times t. Here, $u(\mathbf{x}, t)$ denotes the PDE solution of the problem and $u_h(\mathbf{x}, t)$ the FEM solution. The mesh size of the FEM mesh is denoted by h, λ is the convergence order of the FEM, and C is a constant independent of λ. For problems with a smooth right-hand side $f \in L^2(\Omega)$, classical theory guarantees (under various other necessary assumptions) $\lambda = 2$ for all spatial domains, in particular in $d = 2$ and 3 dimensions. There are many sources for this results, including [3, 6].



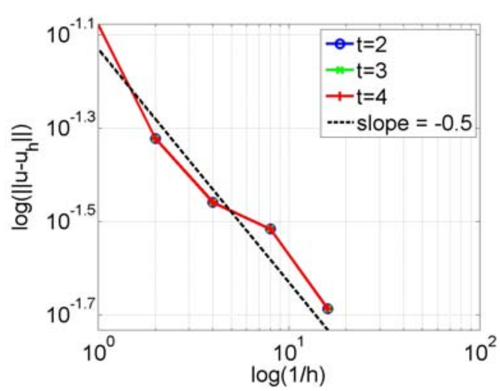
(a) $d = 2$



(a) $d = 2$



(b) $d = 3$



(b) $d = 3$

Figure 1: Smooth test problem: log(error-norm) vs. $\log(1/h)$.

Figure 2: Non-smooth test problem: log(error-norm) vs. $\log(1/h)$.

But if f is not smooth, for instance if it is a point source modeled by a Dirac delta function $f = \delta(\mathbf{x})$, classical theory does not apply any more, since $f \notin L^2(\Omega)$. To appreciate the issue, consider that the FEM is perfectly suited to implement a Dirac delta function, as explained in instructions in the COMSOL User's Guide on how to add a point source. Rigorous estimates have been available for the corresponding stationary elliptic problem as far back as [4], but have been missing for the time-dependent parabolic problem (1.1), even in its simple linear form. We have just recently been able to extend the rigorous theory to this type of problem now and used COMSOL Multiphysics for the numerical studies [5]. The result shows that the convergence order λ in (1.4) depends on the spatial dimension d now and is $\lambda = 2 - d/2$ for spatial domains $d = 2$ and 3, that is, $\lambda = 1$ for $d = 2$ and $\lambda = 0.5$ for $d = 3$.

A powerful way to visualize the result of convergence studies such as the ones needed to confirm analytic results like (1.4) is a log-log plot of the error on the left-hand side of (1.4) vs. the reciprocal of the mesh spacing, $1/h$. The reciprocal of h is used here, so that decreasing the mesh size is equivalent to moving to the right on the horizontal axis. In this form, the estimate (1.4) plots as a line with its slope being the negative of the convergence order λ. Figures 1 (a) and (b) show plots of this type for a smooth test problem, with $f \in L^2(\Omega)$, for dimensions $d = 2$ and 3, respectively. The theoretically predicted slopes of -2 in both cases are shown as dashed lines. The three solid lines show observed convergence orders at three points in time $t = 2, 3, 4$, which clearly confirm the theoretical prediction. Figures 2 (a) and (b) show the analogous plots for a non-smooth test problem, with $f = \delta(\mathbf{x})$ modeling a point source, for dimensions $d = 2$ and 3, respectively. The theoretically predicted slopes of -1 and -0.5, respectively, are again shown as dashed lines, in clear agreement with the observed solid lines.

COMSOL Multiphysics is an excellent tool for numerical studies of this type, because it can readily implement a point source, has reliable time-stepping, accurate linear solvers, and the process of refining the mesh repeatedly is easily automated through the use of LiveLink with MATLAB. But the process has some pitfalls, and this paper therefore presents some information on the techniques needed in COMSOL 4.2 to enable the studies, including how to correctly implement the Dirac delta function for a time-dependent problem, how to set up a study with repeated uniform mesh refinement at several points in time as needed for a time-dependent PDE problem, how to use a reference solution since no analytic PDE solution is available, how to collect data from each refinement level and compute the convergence order from them, how to use LiveLink for MATLAB for the convergence study to be carried out in a convenient automated fashion, and more. This work follows previous papers, all on the stationary elliptic analogue to (1.1), starting with [1, 2] for smooth and non-smooth sources, respectively, and [7, 8] providing a tutorial description of the process for COMSOL 4.

2 FEM Theory

One practical test for reliability of a FEM solution is to refine the FEM mesh, compute the solution again on the finer mesh, and compare the solutions on the two meshes qualitatively. The FEM theory provides a quantification of this approach by comparing FEM errors $u - u_h$ involving the PDE solution u compared to the FEM solution, according to (1.4).

We use this theory here for linear Lagrange elements as provided in COMSOL Multiphysics. Since the domain $\Omega = (-1, 1)^d$ has piecewise smooth boundaries, it can be discretized by the triangular meshes in $d = 2$ and by tetrahedral meshes in $d = 3$ dimensions without error. The convergence studies performed rely on a sequence of meshes with mesh spacings h that are halved in each step. This is accomplished by uniformly refining an initial mesh repeatedly, starting from a coarse initial mesh to allow as many refinements as possible. For the initial mesh, we take advantage of the shape of Ω that admits a very coarse, uniform mesh that still includes the origin, where $\delta(\mathbf{x})$ is centered, as a mesh point. In $d = 2$ dimensions, the initial mesh consists of 4 triangles with 5 vertices given by the 4 corners of Ω plus the center point. In $d = 3$ dimensions, the initial mesh has 28 tetrahedra with 15 vertices and is shown in Figure 5 (on page 6). For each of the meshes considered, we track the number of mesh elements, the degrees of freedom (DOF) of the linear nodal elements for that mesh, and the mesh spacing h for each refinement level r from the initial mesh for $r = 0$ to the finest mesh explored, as summarized in Table 3 (on page 6). The solution plots in the following sections use the finest mesh.

For the conditions of the test problem (1.1) on the domain $\Omega = (-1, 1)^d$, the assumptions of the theory are satisfied and the element error is bounded. The convergence studies in the following numerical experiments compute an estimate $\lambda^{(\mathrm{est})}$ to the convergence order λ in (1.4) according to the formula

$$\lambda^{(\mathrm{est})} = \log_2 \left(\frac{\|u_{2h}(\cdot, t) - u(\cdot, t)\|_{L^2(\Omega)}}{\|u_h(\cdot, t) - u(\cdot, t)\|_{L^2(\Omega)}} \right), \quad (2.1)$$

for all times t. Here, u_h denotes the finite element solution on a mesh with mesh spacing h and u_{2h} on a mesh with twice the mesh spacing. Formula (2.1) is derived by assuming equality in (1.4) and applying it both to u_h and u_{2h}, then forming their ratios and solving for λ. In (2.1), the notation u denotes the PDE solution of (1.1).

If the PDE solution is not available in analytic form, the convergence study can still be carried out by using the FEM solution on the finest mesh as so-called reference solution. This is the standard approach in the case that the PDE solution is not available and is necessary, for instance, for non-smooth problems that do not admit an analytic solution. To use this approach in COMSOL, the numerical solution for each mesh refinement r is exported as a data file for the times of interest. The numerical solution is computed on the highest refined mesh which we treat as a reference mesh. The solutions for the lower refined meshes are imported for comparison on this reference mesh through the use of COMSOL's built-in interpolation function. Using the post-processing tools, we can compute the error. The entire process is easily automated through the use of LiveLink with MATLAB.

3 Smooth Test Problem

To validate our numerical estimation procedure, we first consider a smooth test problem, for which the solution $u(\mathbf{x}, t)$ is both available in analytical form and smooth. Specifically, we choose in (1.1) the source term $f(\mathbf{x}, t)$ such that the problem (1.1) admits the analytic PDE solution

$$u(\mathbf{x}, t) = \left(1 - e^{-t^2/4}\right) \cos^2\left(\frac{\pi x_1}{2}\right) \cos^2\left(\frac{\pi x_2}{2}\right).$$

The solution exhibits its most significant transient in time from about $1 \leq t \leq 4$. Therefore, we analyze the error bound (1.4) at the times $t = 2$, 3, and 4. To check the solution qualitatively, we plot the numerical solution $u_h(\mathbf{x}, t)$ vs. $\mathbf{x}$ of the two-dimensional problem at various times as shown in Figure 3, which shows the expected behavior of the PDE solution $u(\mathbf{x}, t)$.

To check the solution quantitatively, Table 1 lists for each refinement level r the error $\|u_h(\cdot, t) - u(\cdot, t)\|_{L^2(\Omega)}$ of (1.4) and in parentheses the estimate λ^{est} according to (2.1) at time $t = 3$; similar data was obtained for $t = 2$ and 4. We observe that the value of $\lambda^{(est)}$ approaches the value 2, which is expected for a smooth source term. This data provides the basis for the graphical visualization in the log-log plot in Figure 1.

Since the non-smooth problem does not have a known PDE solution, we test the estimation procedure using a reference solution, as explained in Section 2, already for the smooth problem. In fact, the data in Table 1 and Figure 1 is based on that approach; the original approach using the known PDE solution gives equivalent results.

Table 1: Convergence studies for the smooth test problem on triangular meshes using reference solution in dimensions $d = 2$ and 3.

r	$t = 3$
0	1.333e-01
1	7.395e-02 (0.85)
2	4.046e-02 (0.87)
3	1.029e-02 (1.98)
4	2.579e-03 (2.00)
5	6.290e-04 (2.04)

(a) $d = 2$

r	$t = 3$
0	9.531e-02
1	6.621e-02 (0.53)
2	2.107e-02 (1.65)
3	5.669e-03 (1.89)
4	1.511e-03 (1.91)

(b) $d = 3$

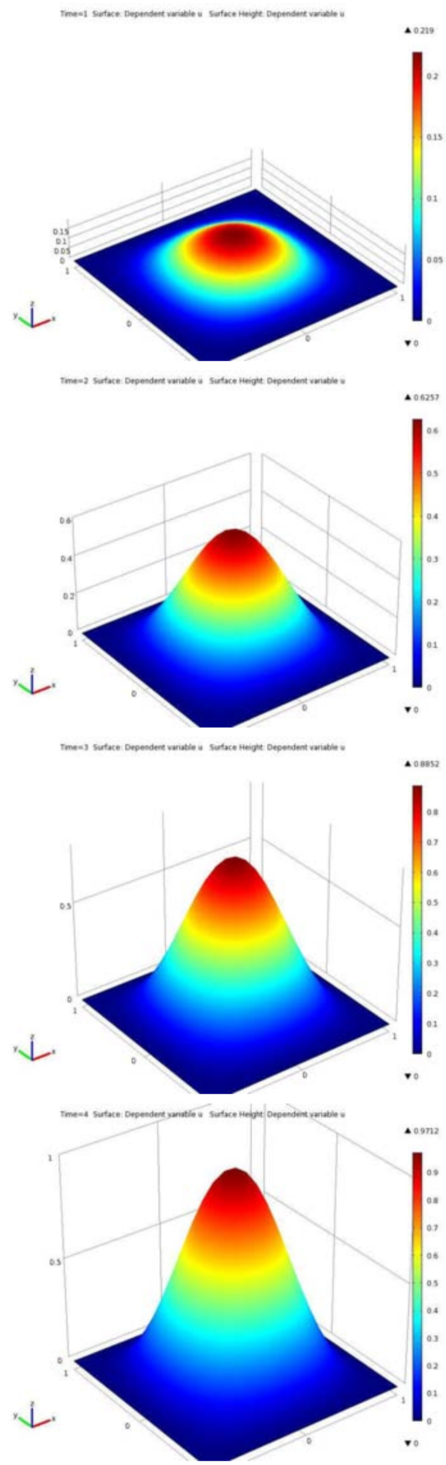


Figure 3: Numerical solutions for the smooth test problem $t = 1, 2, 3, 4$

4 Non-Smooth Test Problem

In the case of the non-smooth test problem, the source term is provided by the Dirac delta function $f(\mathbf{x}, t) = \delta(\mathbf{x})$ and has been positioned at the center of the domain. On physical grounds, it is clear that the solution, starting from the initial condition $u = 0$, will grow dramatically due to the injection of mass at the center for all times $t > 0$. The qualitative check on the solution behavior in Figure 4 shows the dramatic spike at the center of domain that results from the continued injection. The implementation of the delta function in COMSOL makes use of the instructions in the User's Guide on how to add a point source. However, for a time-dependent problem, it is necessary to multiply the basis function by the Boolean operator `(t>0)` to ensure that at $t = 0$ the initial value of u is truly zero over the domain $\overline{\Omega}$.

Unlike the smooth problem, we do not have a PDE solution for comparison so we make use of the numerical solution on the finest mesh as a reference solution, as explained in Section 2. We again investigate the three times $t = 2$, 3, and 4. Table 2 present the error based on the reference solution as well as the observed $\lambda^{(est)}$. For $d = 2$ dimensions in Table 2 (a), we see that $\lambda^{(est)}$ approaches the value of 1, while for $d = 3$ dimensions in Table 2 (b), it approaches the value of 0.5. This is in agreement with the theory in [5], which predicts that the value should be $2 - d/2$ for d dimensions. These data are again the basis for the graphical visualization in the log-log plots in Figure 2.

Table 2: Convergence studies for the non-smooth test problem on triangular meshes using reference solution in dimensions $d = 2$ and 3.

r	$t = 3$
0	3.433e-02
1	2.286e-02 (0.59)
2	1.158e-02 (0.98)
3	5.839e-03 (0.99)
4	2.815e-03 (1.05)
5	1.307e-03 (1.11)

(a) $d = 2$

r	$t = 3$
0	8.363e-02
1	4.761e-02 (0.81)
2	3.477e-02 (0.45)
3	3.049e-02 (0.19)
4	2.057e-02 (0.57)

(b) $d = 3$

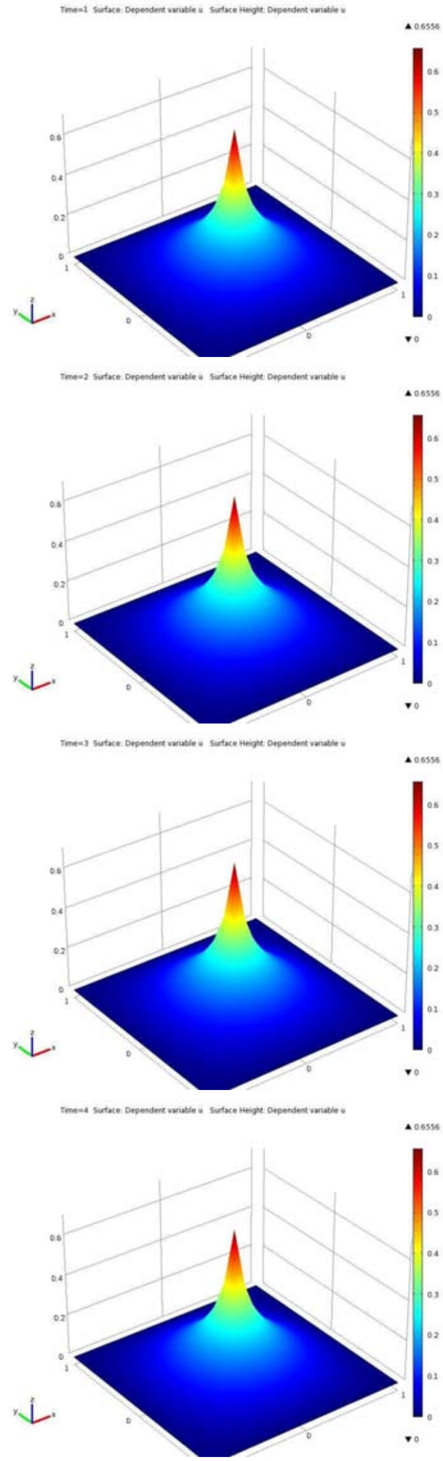


Figure 4: Numerical solutions for the non-smooth test problem $t = 1, 2, 3, 4$

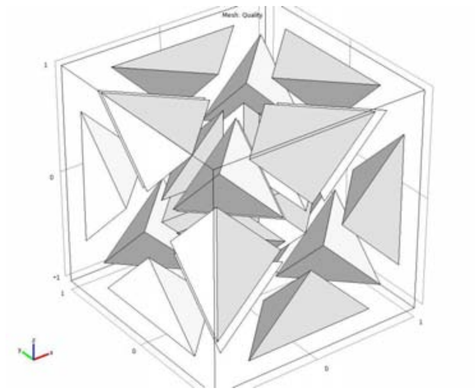


Figure 5: Exploded view of the initial mesh in $d = 3$ dimensions.

Table 3: Finite element data for all meshes in dimensions $d = 2$ and 3 for all refinement levels r.

(a) $d = 2$			
r	N_e	$N =$ DOF	$\max_e h_e$
0	4	5	2.000000
1	16	13	1.000000
2	64	41	0.500000
3	256	145	0.250000
4	1024	545	0.125000
5	4096	2113	0.062500
6	16384	8321	0.031250
(b) $d = 3$			
r	N_e	$N =$ DOF	$\max_e h_e$
0	28	15	2.000000
1	224	69	1.000000
2	1792	409	0.500000
3	14336	2801	0.250000
4	114688	20705	0.125000
5	917504	159169	0.062500

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