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

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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

$$u_t - \nabla \cdot \nabla u = f \quad \text{for } x \in \Omega \text{ and } 0 < t \leq T, \tag{1}$$

$$u = 0 \quad \text{for } x \in \partial\Omega \text{ and } 0 < t \leq T, \tag{2}$$

$$u = 0 \quad \text{for } x \in \overline{\Omega} \text{ at } t = 0, \tag{3}$$

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

$$\|u(\cdot,t) - u_h(\cdot,t)\|_{L^2(\Omega)} \leq C\, h^{\lambda}, \quad \text{as } h \to 0, \text{ for all times } t. \tag{4}$$

- $u(\mathbf{x},t)$ denotes the PDE solution of the problem and $u_h(\mathbf{x},t)$ the FEM solution
- h is the mesh size of the FEM mesh
- λ is the convergence order of the FEM
- C is a constant independent of λ.

A Priori Error Estimate

$$\|u(\cdot,t) - u_h(\cdot,t)\|_{L^2(\Omega)} \le C\, h^{\lambda} \quad \text{as } h \to 0, \text{ for all times } t$$

- For problems with a smooth right-hand side $f \in L^2(\Omega)$ in $u_t - \nabla \cdot \nabla u = f$, classical theory guarantees $\lambda = 2$ for all spatial domains, in particular in $d = 2$ and 3 dimensions. [e.g., Thomeé 2006, Quarteroni and Valli 1994].
- If f is not smooth, e.g., if it is a point source modeled by a Dirac delta distribution $f = \delta(\mathbf{x})$, classical theory does not apply.
  - A new extension to the rigorous theory has been worked out for this type of problem and COMSOL Multiphysics was used for the numerical studies. The result shows that the convergence order λ depends on the spatial dimension d, in this case, and is given by $\lambda = 2 - d/2$.
    [Seidman, Gobbert, Trott, and Kružík, *Numer. Math.*, submitted].

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.

$$\lambda^{(\text{est})} = \log_2 \left(\frac{\| u_{2h}(\cdot, t) - u(\cdot, t) \|_{L^2(\Omega)}}{\| u_h(\cdot, t) - u(\cdot, t) \|_{L^2(\Omega)}} \right), \quad \text{for all times } t. \qquad (5)$$

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.

Use of COMSOL Multiphysics:

- Linear Lagrange elements as provided in COMSOL Multiphysics
- The domain $\Omega = (-1, 1)^d$ has piecewise smooth boundaries can be discretized without error
    - Triangular meshes in $d = 2$
    - Tetrahedral meshes in $d = 3$
- Convergence studies performed rely on a sequence of meshes with mesh spacings h that are halved in each step.
    - 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.
    - 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

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.

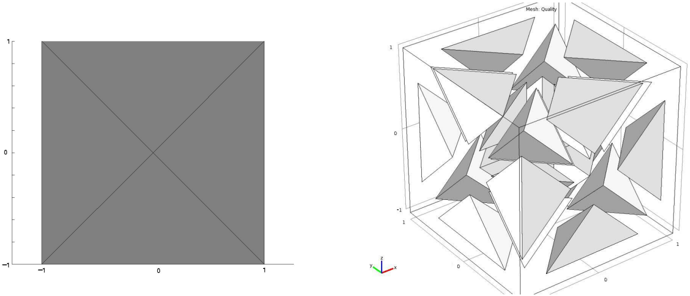

Figure 1: Initial mesh for $d = 2, 3$

Table 1: Finite element data for all meshes in two and three dimensions for all refinement levels r.

(a) Two spatial dimensions on a triangular mesh			
r	N_e	$N = \text{DOF}$	$\max_e h_e$
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) Three spatial dimensions on a tetragonal mesh			
r	N_e	$N = \text{DOF}$	$\max_e h_e$
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

Smooth Problem

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 the source term $f(\mathbf{x}, t)$ such that the problem admits the analytic PDE solution

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

- Solution exhibits its most significant transient in time from about $1 \leq t \leq 4$. Therefore, we analyze the error bound at the times $t = 2$, 3, and 4.
- While the smooth problem does have a known PDE solution, the non-smooth problem does not. So, we test the estimation procedure on the smooth problem as well using a reference solution: $r_{\text{ref}} = 6$ for dimensions $d = 2$ and $r_{\text{ref}} = 5$ for $d = 3$.

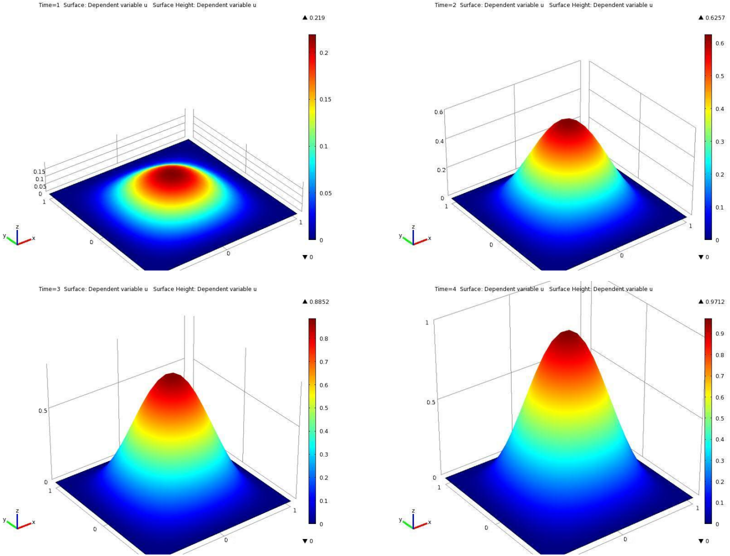

Figure 2: Numerical solutions for the smooth test problem $t = 1, 2, 3, 4$

Table 2: Convergence studies in two dimensions ($d = 2$) for the smooth test problem on triangular meshes.

(a) Smooth problem: true error			
r	$t = 2$	$t = 3$	$t = 4$
0	9.385e-02	1.333e-01	1.465e-01
1	5.196e-02 (0.85)	7.398e-02 (0.85)	8.136e-02 (0.85)
2	2.848e-02 (0.87)	4.048e-02 (0.87)	4.450e-02 (0.87)
3	7.249e-03 (1.97)	1.032e-02 (1.97)	1.134e-02 (1.97)
4	1.833e-03 (1.98)	2.609e-03 (1.98)	2.870e-03 (1.98)
5	4.628e-04 (1.99)	6.589e-04 (1.99)	7.246e-04 (1.99)
(b) Smooth problem: reference error			
r	$t = 2$	$t = 3$	$t = 4$
0	9.385e-02	1.333e-01	1.465e-01
1	5.194e-02 (0.85)	7.395e-02 (0.85)	8.133e-02 (0.85)
2	2.846e-02 (0.87)	4.046e-02 (0.87)	4.446e-02 (0.87)
3	7.228e-03 (1.98)	1.029e-02 (1.98)	1.131e-02 (1.97)
4	1.812e-03 (2.00)	2.579e-03 (2.00)	2.836e-03 (2.00)
5	4.419e-04 (2.04)	6.290e-04 (2.04)	6.916e-04 (2.04)

Table 3: Convergence studies in three dimensions ($d = 3$) for the smooth test problem on tetragonal meshes.

(a) Smooth problem: true error			
r	$t = 2$	$t = 3$	$t = 4$
0	6.707e-02	9.531e-02	1.047e-01
1	4.664e-02 (0.52)	6.621e-02 (0.53)	7.273e-02 (0.53)
2	1.483e-02 (1.65)	2.107e-02 (1.65)	2.315e-02 (1.65)
3	3.987e-03 (1.90)	5.669e-03 (1.89)	6.226e-03 (1.89)
4	1.063e-03 (1.91)	1.511e-03 (1.91)	1.656e-03 (1.91)
(b) Smooth problem: reference error			
r	$t = 2$	$t = 3$	$t = 4$
0	6.691e-02	9.508e-02	1.045e-01
1	4.642e-02 (0.53)	6.590e-02 (0.53)	7.239e-02 (0.53)
2	1.461e-02 (1.67)	2.075e-02 (1.67)	2.281e-02 (1.67)
3	3.759e-03 (1.96)	5.343e-03 (1.96)	5.873e-03 (1.96)
4	8.380e-04 (2.17)	1.190e-03 (2.17)	1.308e-03 (2.17)

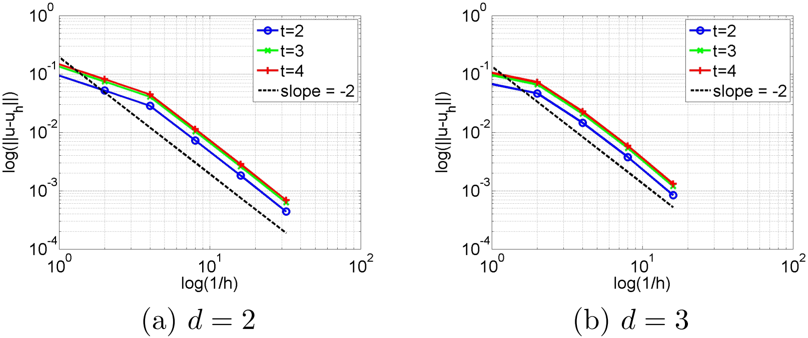

Figure 3: Smooth test problem: log(error-norm) vs. $\log(1/h)$.

- Computational tests confirm the convergence order $\lambda = 2$ *independent of dimension* $d = 2$ *or* 3.

Non-Smooth Problem

In the case of the non-smooth test problem, the source term is provided by the Dirac delta distribution $f(\mathbf{x}, t) = \delta(\mathbf{x})$ and has been positioned at the center of the domain.

- 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 implementation of the delta distribution 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 $\overline{\Omega}$.
- 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

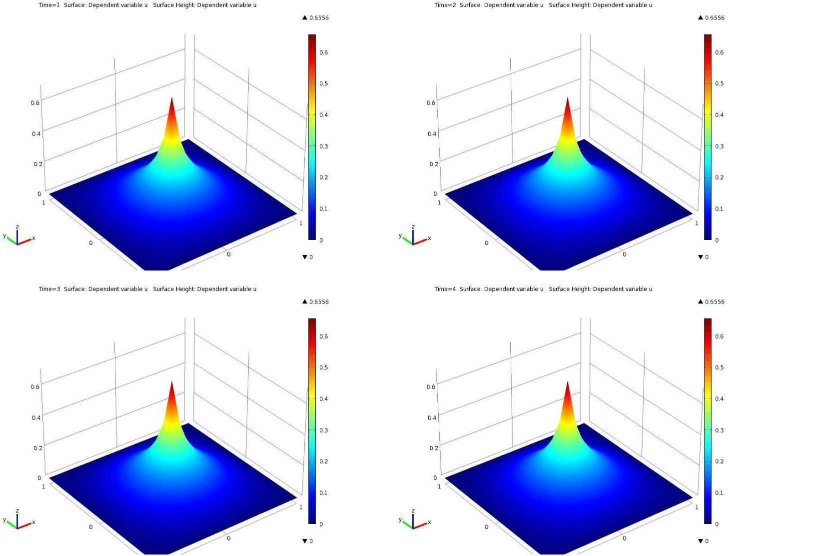

Figure 4: Numerical solutions for the Non-Smooth test problem $t = 1, 2, 3, 4$

Table 4: Convergence studies for the Non-Smooth test problem.

(a) Non-Smooth problem $d = 2$: reference error			
r	$t = 2$	$t = 3$	$t = 4$
0	3.419e-02	3.433e-02	3.433e-02
1	2.271e-02 (0.59)	2.286e-02 (0.59)	2.286e-02 (0.59)
2	1.138e-02 (1.00)	1.158e-02 (0.98)	1.158e-02 (0.98)
3	5.615e-03 (1.02)	5.839e-03 (0.99)	5.839e-03 (0.99)
4	2.613e-03 (1.10)	2.815e-03 (1.05)	2.815e-03 (1.05)
5	1.193e-03 (1.13)	1.307e-03 (1.11)	1.307e-03 (1.11)
(b) Non-Smooth problem $d = 3$: reference error			
r	$t = 2$	$t = 3$	$t = 4$
0	8.363e-02	8.363e-02	8.363e-02
1	4.761e-02 (0.81)	4.761e-02 (0.81)	4.761e-02 (0.81)
2	3.477e-02 (0.45)	3.477e-02 (0.45)	3.477e-02 (0.45)
3	3.049e-02 (0.19)	3.049e-02 (0.19)	3.049e-02 (0.19)
4	2.057e-02 (0.57)	2.057e-02 (0.57)	2.057e-02 (0.57)

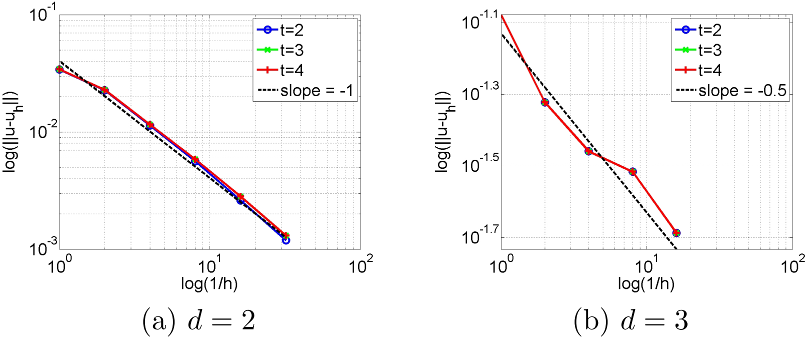

Figure 5: Non-smooth test problem: log(error-norm) vs. $\log(1/h)$.

- Computational tests confirm the convergence order $\lambda = 2 - d/2$ *dependent on dimension* d: $\lambda = 1$ for $d = 2$ and $\lambda = 0.5$ for $d = 3$, as proved in [Seidman, Gobbert, Trott, and Kružík, *Numer. Math.*, submitted].

Conclusions:

- 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.
- Using COMSOL, we were able to provide numerical studies to support new theoretical results which showed that for non-smooth problems of the type discussed, the rate of convergence $\lambda = 2 - d/2$ [Seidman, Gobbert, Trott, and Kružík, *Numer. Math.*, submitted]