Accuracy Tests for COMSOL - and Delaunay Meshes

E. Holzbecher*, Hang Si
Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin (GERMANY)
Mohrenstr. 39, 10117 Berlin, GERMANY
*Corresponding author: holzbecher@wias-berlin.de

Abstract: In the paper we examine the accuracy of various meshes for different model regions and simple differential equations in 2D and in 3D. We study the potential equation for a single irregular domain (2D testcase 1), for a simple domain with irregular sub-domains (2D testcase 2) and a 3D testcase. For testcase 1 we compare with the analytical solution, for testcases 2 with the best solution, obtained by several adaptive grid refinements on a fine mesh. We study meshes obtained by global refinements and by adaptive grid refinement, using various options available in COMSOL Multiphysics. For quadratic elements we find convergence rates between 1 and 1.5, i.e. significantly reduced in comparison to the theoretical rate. Moreover, for testcase 1 we examine imported meshes with Delaunay property and find no advantages in comparison to non-Delaunay meshes for the chosen set-up.

Keywords: mesh refinement, adaptive meshes, Laplace equation, potential flow, convergence rate, mesh quality, Delaunay mesh,

1. Introduction

The accuracy of a numerical solution for a given level of grid refinement depends, among other factors, on the mesh quality.
We examine two test problems for the Laplace equation, one in 2D and one in 3D, as a classical partial differential equation and a generalized problem with an inhomogeneous material property. Both test problems represent typical problem constellations with applications in various fields, from electrostatics, porous media flow to fluid dynamics.
We explore various model approaches, concerning Lagrange Finite Element, and meshing techniques. We demonstrate the gain from using adaptive meshing. We also compare with theoretical results: for most models the convergence order lies between 1 and 1.5 (for default quadratic elements), i.e. between a linear and a quadratic increase of accuracy with the spatial grid size. Moreover we explore models with imported Delaunay meshes.

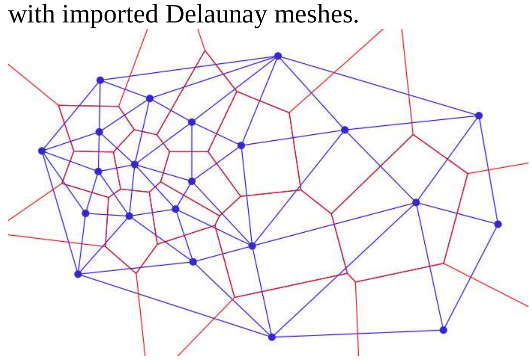

Figure 1: Sketch of a Delaunay mesh and Voronoi diagram

A special mesh is called Delaunay mesh whose elements satisfying the Delaunay criterion (also called the "empty sphere criterion"). Let *V* be a finite set of vertices in $\mathbb{R}^d$. A simplex σ in *V* is called *Delaunay* if it has a circumscribed sphere such that no vertex of *V* lies inside it. A *Delaunay triangulation* for *V* consists of Delaunay simplices in *V* (Delaunay 1934). Delaunay triangulation has many optimal geometrical properties (Rajan 1994). For example, it's dual is a Voronoi diagram. Their relation is shown in Figure 1. In 2D, if no 4 vertices of *V* share a common sphere, the Delaunay triangulation of *V* is unique, and it maximizes the minimum angle among all other possible triangulations of *V*. In function interpolation, the Delaunay triangulation minimizes the interpolation error among all other triangulations of the same set of vertices.

2. Convergence and Order Mesh Quality

The convergence order ϑ is defined by the relationship

$$\|e\| = O\left(h^{\vartheta}\right) \tag{1}$$

where *e* denotes the error, $\|..\|$ a norm, and *h* the typical element size. The convergence order is a measure for the improvement of the solution as a consequence of mesh refinement.

In order to determine the convergence order from numerical runs, the errors of runs with different refinement level have to be related. For irregular meshes, instead of the mean element size one may alternatively use the degrees of freedom (DOF) for the determination of the convergence rate. The mean grid spacing h decreases with number of DOF. Jänicke & Kost (1996, 1999) use the formula

$$\vartheta = -2\frac{\ln\left(\|e_1\|\right)-\ln\left(\|e_2\|\right)}{\ln\left(DOF_1\right)-\ln\left(DOF_2\right)} \qquad (2)$$

where subscripts denote run number. Formula (2) is valid for 2D problems and has to be replaced by corresponding formulae for 1D or 3D problems (Bradji & Holzbecher 2008).

The convergence of a numerical solution of one or several partial differential equations generally depends on various characteristics of the problem, on the numerical algorithm, on the mesh refinement and on the mesh quality.

There are two mesh quality measures calculated by COMSOL. The *element quality* q for a triangle is obtained by:

$$q = \frac{4\sqrt{3}A}{h_1^2+h_2^2+h_3^2} \qquad (3)$$

where A denotes the area, and h_1, h_2 and h_3 the sidelengths. For an 'optimal' equilateral triangle q becomes 1 and is less, but positive, otherwise. A measure for the mesh is the minimum element quality. The other quality measure, reported by COMSOL, is the element area ratio. In the following we only refer to the q-measure, as defined by formula (3). In 3D, for a tetrahedron the quality measure is evaluated using the formula

$$q = \frac{72\sqrt{3}V}{\left(h_1^2+h_2^2+h_3^2+h_4^2+h_5^2+h_6^2\right)^{3/2}} \qquad (4)$$

where V denotes the volume, and the h's the edge lengths.

3. Test-cases

3.1 2D Testcase 1

The first test problem concerns the Laplace equation

$$\nabla^2 u = 0 \qquad (5)$$

Equation (5) may be used for several types of applications. u may represent the hydraulic potential of Darcy flow in porous media or of potential flow in general, or the electric potential in a problem of electrostatics. The unknown variable u may also represent the steady state concentration distribution for a diffusion problem between two reservoirs at constant values or stand temperature in a heat conduction problem.

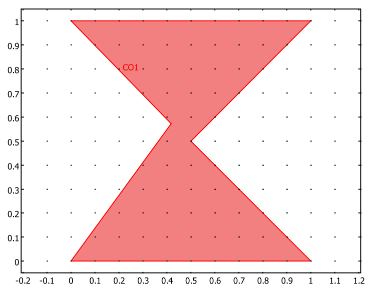

Figure 2: Sketch of model regions for testcase 1

The colored part of Figure 2 shows the model region for testcase 1. There are boundary conditions of Dirichlet type at the upper and lower sides of the shown geometry and Neumann type conditions at all other boundaries. The constriction of the region geometry in the center part is a challenge for the numerical algorithm, as the solution shows steep gradients there, while the gradients near the top and bottom boundary are marginal in relation.

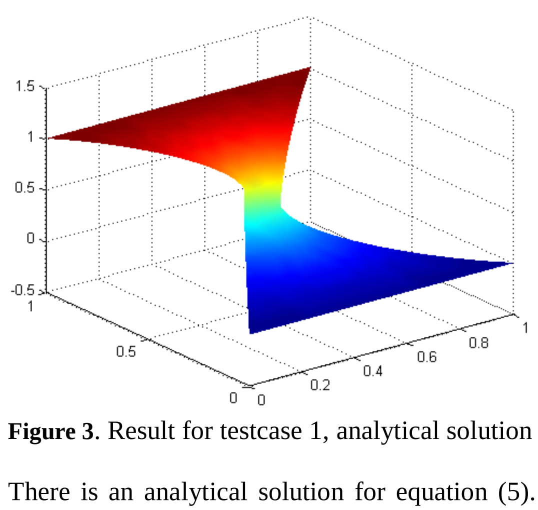

Figure 3. Result for testcase 1, analytical solution

There is an analytical solution for equation (5). This can be obtained from Schwarz-Christoffel mapping to an rectangle (Driscoll & Trefethen

2002). For that purpose we use the Schwarz–Christoffel toolbox (Driscoll 1996), implemented in MATLAB®. A surface plot of the solution is given in Figure 3.
The initial mesh consists of 506 elements and is refined four times by regular refinement, where the no. of elements increases by a factor of 4 by each refinement. The minimum quality index for all simulations is 0.701, and the element area ratio is 0.21.
For all meshes the error in least square-norm is evaluated on the same coarse triangulation of the model region. An overview on the meshes, the errors and the resulting convergence rates is given in Table 1.

Table 1: Results for the testcase 1, default settings (i.e. quadratic elements)

Refine-ments	**DOF**	**No. elements**	$\|e\|_2$ **10^4**	ϑ	
0	1085	506	301	1.25	
1	4193	2024	129		0.91
2	16481	8096	69	0.94	
3	65345	32384	36		2.97
4	260225	129536	13		

Except from the last refinement step, the convergence order lies around 1, which is significantly below the theoretical value of 2 (Ciarlet 1991). This can clearly be attributed to the constriction of the model geometry..
Further runs were performed in order to check Delaunay meshes. Delaunay meshes are not (yet) an option in COMSOL, and have to be produced by other software. For our computations we chose the 'triangle' code (Shewchuk 2008).
Tables 2 to 4 show results for Delaunay meshes of different resolution, produced by the 'triangle' code; Table 2 for linear and Tables 3 and 4 for quadratic elements. The meshes were imported into COMSOL using the converter-code 'readtri' of J. Krause (2006), written in MATLAB (2007). The minimum quality ratio lies at 0.41, except for the finest mesh, where it increases to 0.44. The element area ratio decreases from 0.364 for the coarsest mesh to 0.305 for the finest mesh. 'Triangle' was used with default options (pa) first. Meshes of improved quality were produced with the –D option, and the option to restrict angles to 30° (q-option).

Table 2: Results for the testcase 1, Delaunay mesh, linear elements, COMSOL 3.3

Mean elem. size	**DOF**	**No. elements**	$\|e\|_2$ **10^4**
10^{-3}	466	833	27000
$10^{-3}/2$	917	1693	580
$10^{-3}/4$	1788	3375	388
$10^{-3}/8$	3529	6783	271

Table 3: Results for the testcase 1, default Delaunay mesh, quadr. elements, COMSOL 3.3

Mean elem. size	**DOF**	**No. elements**	$\|e\|_2$ **10^4**
10^{-3}	1764	833	26897
$10^{-3}/2$	3526	1693	126
$10^{-3}/4$	6950	3375	101
$10^{-3}/8$	13840	6783	78

The coarse mesh simulations with Delaunay meshes deliver poor results, which are significantly improved on the next finer mesh. However, tests with further refined meshes give poor improvement rates for Delaunay meshes. This observation holds for linear and quadratic elements. The convergence rates, using Delaunay meshes, are much smaller than those with default COMSOL regular mesh refinements.
The reason for the poor performance of the Delaunay meshing can probably be attributed to the fact that the meshing procedure is less adapted to the special structure of the examined test-case, i.e the constriction of the domain. They are much more oriented to cover the entire domain with triangles of similar size and quality. This is done at each refinement level again, as the Delaunay property is not inherited to finer meshes by using regular grid refinement. COMSOL, in contrast, takes the varying thickness of the domain into account: especially for the coarsest mesh the contrast in element size is high. This high contrast, which is the clue for

highly accurate results, is kept by regular grid refinements, as they were performed in this test.

Table 4: Results for the testcase 1, improved Delaunay mesh (D-option), quadratic elements, COMSOL 3.3, *: last row with q-option in addition.

Mean elem. size	DOF	No. elements	$\lVert e \rVert_2$ 10^4
10^{-3}	1849	854	177
$10^{-3}/2$	3535	1678	133
$10^{-3}/4$	6977	3352	102
$10^{-3}/8$	13805	6728	73
$10^{-3}/8^{*}$	14257	6954	75

Only for smallest DOF high quality meshes ('triangle' q-option) led to more accurate results than the one examined before. For finer meshes the methods deliver only marginally more accurate results.

3.2 2D Testcase 2

The second testcase is 2D also. The material constant σ involved in the differential equation

$$\nabla(\sigma \nabla u) = 0 \qquad (6)$$

is inhomogeneous. A sketch of the model region is given in Figure 4. In the upper and lower white regions σ takes low values (10^{-4} and 10^{-5} respectively), while it is equal to unity in the intermediate (colored) region.

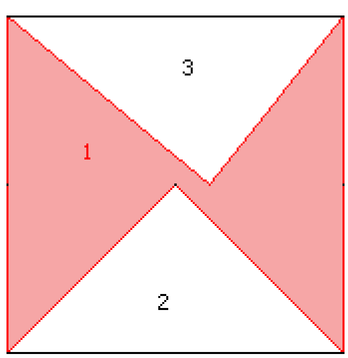

Figure 4: Sketch of model regions within the unit square for testcase 2

Again the problem can be conceived as a simple model study originating from various application fields. In porous media flow σ stands for hydraulic conductivity and the problem considers fluid flow through a system of three different porous media. In electrostatics σ represents the dielectricity of the different media; and in diffusion problems it stands for solute or thermal diffusivity.
There is no analytical solution for this set-up. Therefore we construct a reference soltion, to compare with, by the numerical method. The reference solution is obtained with several default adaptive mesh refinements with quadratic elements. The final mesh is extremely fine in the center of the model region and has 73399 elements and 147072 DOF.

Table 5: Results for the testcase 2 with linear elements

Refine-ments	DOF	No. elements	$\lVert e \rVert_2$ 10^4	ϑ	
0	500	938	2302	1.22	
1	1937	3752	996		1.23
2	7625	15008	433	1.21	
3	30257	60032	188		1.25
4	120545	240128	79		

For all other meshes to be examined the error in L2-norm is evaluated on an equidistant grid with mesh-spacing 1/80.

Table 6: Results for the testcase 2 with quadratic elements

Refine-ments	DOF	No. elements	$\lVert e \rVert_2$ 10^4	ϑ	
0	1937	938	593	1.22	
1	7625	3752	256		1.23
2	30257	15008	110	1.33	
3	120545	60032	44		1.65
4	481217	240128	14		

Table 5 and 6 show results for global mesh refinements using the default options, for linear (Table 5), and for quadratic elements (Table 6). The convergence rate for linear elements lies constantly at about 1.2. The convergence order for the quadratic elements lies only marginally above the order for the linear elements, especially for the first two refinements. It is increasing from one refinement to the next, but still far away from the theoretical value of 2.

In further runs adaptive mesh strategies were examined. A characteristic result is presented in Table 7. It shows that after several adaptive steps the error reduces only slightly. Although the number of elements is more than doubled during the 5th refinement, the accuracy is not improved.

Table 7: Results for testcase 2 with adaptive meshing, linear elements, residual method: weak, refinement method: longest, element selection method: rough global minimum (parameter 1.7)

Refine-ments	**DOF**	**No. elements**	$\|e\|_2$ **10⁴**	ϑ	
0	500	938	2302	3.49	
1	1555	3026	318		1.50
2	4064	8002	155	0.28	
3	9729	19268	137		-
4	21797	43318	132	-	
5	46840	93313	132		

After only two adaptive refinements with a mesh of only 8000 elements a higher accuracy is reached than with a mesh of more than 60000 elements, obtained by global refinement. However with the following mesh refinements the comparative advantage of the adaptive meshing becomes much smaller.

Before continuation with a similar study for quadratic elements, various options for mesh refinement were checked. For adaptive grid refinements we examined various combinations of residual and refinement methods. For the first two refinements of the coarse mesh the results are compared in Table 7. The meshes are refined most by the 'longest' refinement method. After two refinements the same accuracy is reached by all examined variants, but with different mehs sizes. From the observation the 'regular' refinement method, combined with 'coefficient' residual method can be evaluated to be best for the testcase.

The results of an examination study of adaptive mesh refinements for quadratic elements are given in Table 9. Obviously higher order elements perform better with adaptive refinements. The accuracy improves up to the 11th refinement. With further refinements no further improvement is obtained, although the mesh increase factor is highest.

Table 8: Results for testcase 2, adaptive refinements for quadratic elements, selection method: rough global minimum (parameter 1.7)

Refine-ments	**Residual method**	**Refinem. method**	**DOF**	**No. elements**	$\|e_u\|_2$ **10⁴**
1	weak	longest	6971	3454	21
2	weak	longest	21840	10867	7
1	weak	regular	5505	2722	45
2	weak	regular	14395	7152	7
1	coeff.	regular	5107	2522	45
2	"	regular	12749	6326	7

Altogether we reach the same conclusion, as for the linear elements: after a certain number of adaptive refinements the solution does not increase. However, the gain from the adaptive strategy is convincing: a better accuracy is obtained with a mesh consisting of 1566 elements than with a mesh of more than 240000 elements using a global refinement strategy (compare Table 6).

Table 9: Results for testcase 2 for quadratic elements, residual method: coefficient, refinement method: regular, element selection method: fraction of worst error (parameter 0.5)

Refine-ments	**DOF**	**No. elements**	**Mesh increase**	$\|e\|$
1	1997	968	1.032	284
2	2089	1014	1.048	133
3	2133	1036	1.022	125
4	2185	1062	1.025	64
5	2301	1120	1.055	55
6	2401	1170	1.045	35
7	2517	1228	1.050	24
8	2577	1258	1.024	21
9	2773	1356	1.078	20
10	2973	1456	1.074	12
11	3193	1566	1.076	10
12	3505	1722	1.100	10
13	3829	1884	1.094	10

3.3 3D Testcase

Take the triangle with positions (0,0), (-1,-1) and (-1,0) in (x,y) axis for z=0; extrude in z-direction to level z=1 and twist at the same time by α= 165° (=11π/12). The resulting 3D domain is narrow near the middle level of *z*=0.5, compared to the 'ends' at *z*=0 and *z*=1. If one applies a potential difference (again 0 and 1), and sets all other boundaries to isolators (no flow Neumann condition), one obtains a potential field that has almost no gradient near the ends. In the middle there are steep gradients.

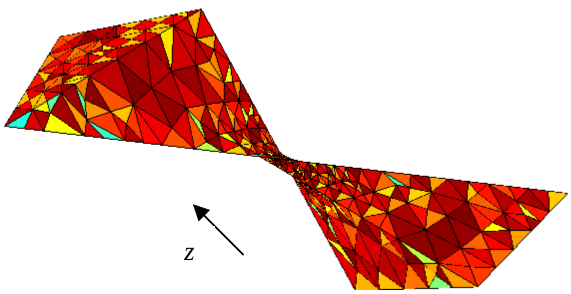

Figure 5: Model region for 3D testcase, with mesh quality visualisation

We examine the potential along the line, which connects the two center points at both ends, given by (-0.5,-0.25) at the *z*=0 level and 0.5*1.118*(cos($\tilde{\alpha}$), sin($\tilde{\alpha}$)) with $\tilde{\alpha}$ =π+.4636-11π/12 at the *z*=1 level. The length 1.118 and the angle .4636 belong to the center line of the original triangle, which connects the origin with the position (-1,-0.5: $\sqrt{1+0.5^2}=1.118$, atan(0.5)=0.4636 (26.565°). The errors, reported in the following are computed from on 400 positions along that line (least squares).

Tables 10 and 11 list the results for the 3D test-case, performed using COMSOL 3.4. We varied the initial mesh, used regular and adaptive mesh refinement strategies and switched the 'quality optimization' option on and off. The list provides mesh quality according to formula (4) and errors. Table 10 lists results for the default FE option with second order Lagrange elements. Table 11 for linear elements. Note that the 'longest' is the default mesh refinement option in 3D!

For coarse meshes, linear element solutions sometimes have less error than quadratic element solutions. However, with grid refinement the performance order changes, as expected. Even, if the convergence order is below the expectation from theory, the improvement with grid refinement is higher for quadratic elements than for linear elements.

Table 10: Results for 3D testcase for quadratic elements.

Mesh & Refine-ments	**DOF**	**Quality optim.**	**No. elements**	**Mesh quality**	$\|e\|_2$ 10^2
extra coarse	381	-	162	0.0846	16.8
coarser	573	-	253	0.0508	12.5
coarse	765	-	352	0.0567	9.72
normal	1461	-	714	0.0561	2.28
fine	2821	-	1492	0.0248	0.79
finer	6668	-	3849	0.0270	0.22
extra fine	18896	-	11801	0.0192	0.09
extra coarse	382	+	161	0.2030	17.9
coarser	572	+	250	0.1934	12.2
coarse	757	+	342	0.0697	9.61
normal	1425	+	676	0.1814	1.69
fine	2736	+	1407	0.2049	0.81
finer	6452	+	3633	0.1954	0.11
extra fine	18158	+	11063	0.2191	0.06
normal & ref.1	4527	-	2636	0.0405	2.10
fine & ref.	9192	-	5578	0.0205	0.57
finer & ref.	23552	-	15155	0.0223	0.078
coarser & ref.	1656	+	880	0.0899	8.85
normal & ref	4289	+	2465	0.1174	2.02
fine & ref.	8686	+	5197	0.1084	0.28
finer & ref.	22415	+	14270	0.1373	0.035
extra fine & ref.	63818	+	42183	0.1404	0.022

Quality optimization is an additional step, which requires computational work only in the mesh mode. The size of the resulting mesh is mostly slightly smaller, while the mesh quality is significantly improved (see column 5)

The gain in mesh quality does not always lead to improved accuracy. Especially for coarse meshes the result for the optimized mesh is sometimes less accurate than the original mesh. However, for fine meshes, optimization pays off (compare 'finer' and 'extra fine' meshes).

Table 11: Results for 3D testcase for linear elements

Mesh & Refine-ments	DOF	Quality optim.	No. elements	Mesh quality	$\|e\|_2$ 10^2
extra coarse	74	-	162	0.0846	2.21
coarser	108	-	253	0.0508	2.21
coarse	140	-	352	0.0567	1.46
normal	255	-	714	0.0561	0.55
fine	464	-	1492	0.0248	0.42
finer	1028	-	3849	0.0270	0.25
extra fine	2726	-	11801	0.0192	0.127
extra coarse	75	+	161	0.2030	2.58
coarser	109	+	250	0.1934	0.90
coarse	141	+	342	0.0697	1.47
normal	256	+	676	0.1814	0.60
fine	464	+	1407	0.2049	0.38
finer	1028	+	3633	0.1954	0.26
extra fine	2726	+	11063	0.2191	0.109
normal & ref.1	732	-	2636	0.0405	3.82
fine & ref.	1436	-	5578	0.0205	3.13
finer & ref.	3510	-	15155	0.0223	1.46
coarser & ref.	286	+	880	0.0899	1.10
normal & ref	697	+	2465	0.1174	0.45
fine & ref.	1368	+	5197	0.1084	0.311
finer & ref.	3357	+	14270	0.1373	0.130
extra fine & ref.	9273	+	42183	0.1404	0.072

4. Summary

- The convergence rate for linear elements is ≈1.2
- For quadratic elements the convergence rate is only slightly increased in comparison to linear elements, and mostly lies significantly below the theoretical value of 2
- In comparison to globally refined meshes adaptive techniques deliver results with same accuracy, but with significantly lower DOF
- Multiple application of adaptive meshing shows reduced improvement with each application
- Delaunay meshes do not offer advantages
- Mesh quality optimization is recommended

5. References

1. Bradji A. & Holzbecher E., On the convergence order of COMSOL solutions, European COMSOL Conference, Grenoble, COMSOL (ed), 2007 (CD-ROM)
2. Bradji A. & Holzbecher E., On the convergence order in Sobolev norms of COMSOL solutions, COMSOL Conference, Budapest, 2008 (to appear)
3. Ciarlet Ph. P., Basic error estimates for elliptic problems, in*: Handbook of Numerical Analysis* **II**, Finite Element Methods (Part 1), P.G. Ciarlet & J.L. Lions (eds.), North-Holand, Amsterdam, 17-352, 1991
4. Delaunay, B. Sur la sphère vide, *Izvestia Akademii Nauk SSSR*, Otdelenie Matematicheskikh i Estestvennykh Nauk **7**, 793—800, 1934
5. Driscoll T.A., A MATLAB toolbox for Schwarz-Christoffel mapping, *ACM Trans. Math. Soft.* **22**, 168-186, 1996
6. Driscoll T.A. & Trefethen L.N., Schwarz-Christoffel mapping, Cambridge Univ. Press, Cambridge, 132p, 2002
7. Jänicke L. & Kost A., Convergence Properties of the Finite Element Method, *IEEE Transactions on Magnetics* **35** (3), 1414-1417, 1999
8. Jänicke L. & Kost A., Error Estimation and Adaptive Mesh Generation in the 2D and 3D Finite Element Method, *IEEE Transactions on Magnetics* **32** (3), 1334-1337, 1996
9. Krause J., personal communication
10. MATLAB®, The Mathworks, http://mathworks.com, 2008
11. Rajan, V. T., Optimality of the Delaunay triangulation in $\mathbb{R}^d$, *Discrete and Computational Geometry* **12**, 189-202, 1994
12. Shewchuk J.R., A two-dimensional quality mesh generator and Delaunay triangulator, http://www.cs.cmu.edu/~quake/triangle.htm, 2008
13. Si H., TetGen - a quality tetrahedral mesh generator and three-dimensional Delaunay triangulator, http://tetgen.berlios.de/, 2008