SCIENTIFIC VISUALIZATION FOR PDES OF 2ND ORDER IV:
COMPARISON BETWEEN THE CONTINUAL AND
THE DISCRETE BOUNDARY VALUE PROBLEM

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Abstract: This paper completes the sequence [3], [4], [5], dedicated to the
scientific visualization of Green’s functions and solutions of initial-value and
boundary-value problems for 2nd order linear PDEs. Here we compare the
continual and the discrete (via finite-difference scheme) initial/boundary problem
for the heat equation in two ways:

- We study the shape of isocurves and the topology of isocurves and iso-
surfaces of the discrete Green’s function and how they depend on the
parameter $\sigma$ which controls the stability and is a measure of the implic-
tness of the difference scheme. The graphical results obtained can be
compared to the graphical results in [4] for the continual Green’s function
of the exact continual initial/boundary problem for the heat equation.

- We study the structure (size and smoothness) of the error of approxima-
tion via the difference scheme as a function of the parameter $\sigma$. Both
stable and unstable cases are considered.

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On the basis of the results obtained some comments and recommendations are made in the concluding section.

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**Key Words:** scientific visualization, heat equation, initial value, boundary value, finite difference scheme, explicit, implicit, Crank-Nicholson difference scheme, backward Euler difference scheme, stability, convergence, Green’s function, continual, discrete, isocurve, colour map, oversmoothing, singularity, computational geometry, computer graphics, applied mathematics

1. Introduction

This work is a continuation of [3] and is the last paper in the sequence of 4 papers (including also [4] and [5]) dedicated to scientific visualization related to initial-value and boundary-value problems for PDEs. Our work on this topic should be considered as extension and upgrade of [6] where we discussed the scientific visualization of the numerical output of the simulator BedSim – see [6] and [3] for further details and references on BedSim.

Our purpose in this paper, as well as in [3], [4] and [5], is to show how our visualization software application discussed in [6] works on data sets generated from PDEs and their numerical approximations.

For the parabolic initial and boundary problem (2) in [3], we compute with high-precision the exact Green’s function (3) in [3] as described in [3], [4]. Further, for sufficiently smooth initial and boundary conditions and RHS in (2), we use the integral representation (4) in [3] of the solution of (2) in [3], as described in [3] and [5]. We consider also the discrete approximation by classical 2-layer difference schemes (see [8]). These difference schemes depend on the step $h$ in the 1D space variable $x$, $\tau$ in the time variable $t$, and on $\sigma \in [0, 1]$ where the parameter $\sigma$ provides a quantitative measure of the implicitness of the difference scheme ($\sigma = 0$ corresponds to the ”purely” explicit scheme, and $\sigma = 1$ corresponds to the ”purely” implicit scheme (see [8])). The formulation of the discrete initial/boundary-value problem is given in (14) of [3]. The discrete Green’s function for this problem is given in (15) and (16) of [3]. The respective discrete-sum representation of the solution of this discrete problem is given in (17), (18) and (19) of [3].
It is known (see [8], Sections 5.1.3–5.1.7, and [2]) that this type of difference schemes are stable (in appropriate mesh-dependent norms, both with respect to initial data and to RHS and boundary-value data) when the steps $h$ and $\tau$ are related with $\sigma$ by

$$0 \leq \sigma_0 \leq \sigma \leq 1,$$

where $\sigma_0$ is $\sigma_\varepsilon$ for $\varepsilon = 0$ in the expression $\sigma_\varepsilon = \frac{1}{2} - \frac{1-\varepsilon}{4\varepsilon} h^2$, $0 \leq \varepsilon \leq 1$. It is also known that, in general, for every $\sigma$ satisfying (1) the rate of local approximation of this difference scheme is $O(h^2 + \tau)$, but in the special case $\sigma = \frac{1}{2} = \sigma_\varepsilon$ for $\varepsilon = 1$ the rate of local approximation improves for $O(h^2 + \tau^2)$, and in the special case

$$\sigma^* = \frac{1}{2} - \frac{h^2}{12\tau} = \sigma_\varepsilon, \quad \text{for} \quad \varepsilon = \frac{2}{3},$$

the difference scheme has increased rate of local approximation $O(h^4 + \tau^2)$ for appropriately chosen RHS of the difference scheme, if the RHS in (2) of [3] is sufficiently smooth (see [8], Section 5.1.3). Moreover, the schemes with $\sigma = \frac{1}{2}$, $\sigma^*$ are stable, since it is easy to see that $\sigma = \frac{1}{2}$, $\sigma = \sigma^*$ satisfies (1).

Taking these facts into consideration, we shall visualize (see also Section 3 of [3]):

- The error of approximation of the exact continual Green’s function by the discrete Green’s function for fixed $h$, $\tau$ and varying $\sigma$ (when (1) is fulfilled) with special attention to the boundary case between stability and instability, $\sigma = \sigma_0$, which is stable, but interesting additional phenomena are observed due to the numerical round-up errors. For this visualization we shall use isosurfaces in 3D and, and colour (mode 1) mapping of the values (see the sequel of this section for orientation into the visualization techniques used). See Section 2.

- For several representative values of $\sigma$ (including both stable and unstable cases), the error of approximation on the mesh of the exact continual solution of the boundary problem by the discrete solution of the finite difference scheme (visualized as a functional surface in 3D and via a colour (mode 1) map). See Section 3.

The derivation of the formulae from [3] mentioned so fare is discussed in Appendices A.1, B.1 and C.1 of [3], while their approximate numerical computation is discussed in Section 3 of [3].

The types of visualization techniques (in 3D and in variable dimensions, including higher than 3, via colour (mode 1, 2 and 3) mapping) is discussed in
Section 2 of [3]. Also in this section of [3] is described our software-application used to obtain the graphical results given in this paper. This is the same software tool which was used for the visualization related to the ODE-based simulator BedSim in [6].

2. Continual Versus Discrete Green’s Function for the Heat Equation

Recall that (see Subsection 4.4 of [3]) for \( \sigma \) we assume \( \sigma \in [0, 1] \) (\( \sigma = 0 \) – explicit scheme; \( \sigma = \frac{1}{2} \) – Crank-Nicholson (implicit) scheme; \( \sigma = 1 \) – backward Euler (fully) implicit scheme)

In Figures 1, 2, 3 and 4 are given the isosurfaces and isocurves of the discrete Green’s function (15), (16) in [3] for an increasing sequence of four respective isovales. For each of these isovales, on the respective figure are given the isosurfaces and isocurves for a decreasing sequence of four representative values of \( \sigma \) for which the difference scheme is stable. The largest of these values is \( \sigma = 1 \), and the smallest is \( \sigma = \sigma_0 \) – the limiting value of \( \sigma \), below which the scheme becomes unstable.

Some observations and comments:

- For \( \sigma = 1 \) (the ”most stable” case) the discrete Green’s function approximates the exact Green’s in an excellent way for the whole range of isovales. In fact, in these figures we have not presented the isosurfaces and isocurves of the exact Green’s function because for all of these figures the exact isosurfaces and isocurves are visually undistinguishable from their approximations for \( \sigma = 1 \).

- As \( \sigma \) decreases from 1 to \( \sigma_0 \), the approximation gradually deteriorates in quality but remains consistent for all \( \sigma \in [\sigma_0, 1] \). The deterioration is in two aspects: deformation of the shape of the isosurfaces and isocurves, and changes in their topology.

- For fixed \( \sigma \in [\sigma_0, 1] \) the deformation of the isosurfaces decreases with the increase of the isovalue.

- For fixed \( \sigma \in [\sigma_0, 1] \) the level of distortion of the topology of isosurfaces and isocurves increases with the increase of the isovalue.

- The limiting case \( \sigma = \sigma_0 \) is the most interesting one, and combines consistent approximation with elements of noise-like chaotic behavior, due
Figure 1: Isosurfaces for the discrete parabolic Green’s function for isovalue $= 0.14$ and different values of $\sigma$. Here all colour maps appear as grey-scale.

to round-up errors. This noise can be observed at the right-hand side of the plots for $\sigma = \sigma_0$ where a distinctive pattern of fractal isocurves appears for very small (positive) isovales. It is typical only for $\sigma = \sigma_0$ and disappears for $\sigma \in (\sigma_0, 1]$.

We study the special effects appearing in the limiting case $\sigma = \sigma_0$ in further detail in Figures 5 and 6.
Some observations and comments:

- For fixed $t - \tau$, the quality of approximation and amount of noise vary greatly for different $x$ and $\xi$, see Figure 5.

- For different values of $t - \tau$ the topology of the isosurfaces and isocurves is very different and changes rapidly with the change of $t - \tau$ (see Figure
Figure 3: Isosurfaces for the discrete parabolic Green’s function for isovalue = 1.7 and different values of $\sigma$. Here all colour maps appear as grey-scale.

where the dependence of the discrete Green’s function on $(x, \xi) \in [0, 1]^2$ and different values of $t - \tau$) is given.
3. Visualization of the Approximation Error

In Figure 7 is given a comparative visualization of the distribution of the absolute error of approximation of the exact solution of the parabolic problem (4) in [3] (more precisely, (5) in [3] with smooth RHS, initial and boundary conditions) via the solution of the difference scheme (17), (18), (19) in [3], as
a function of $\sigma \in [0, 1]$, for fixed $h$ and $\tau$. Note that in Figure 7 the absolute error is scaled to be the same in all four plots. We have considered the two extreme stable cases (a) $\sigma = 1$ ("most stable") and (b) $\sigma = \sigma_0$ ("least stable") an extreme unstable case (d) $\sigma = 0$ and a "less unstable" (but still unstable)
Figure 6: Intersections for different $t$-values for the discrete parabolic Green’s function for $\sigma = \sigma_0$. Here all colour maps appear as grey-scale.

case (c) which is intermediate between (b) and (d).

Some observations and comments:

- Comparing the distribution of the absolute error in the stable cases (a) and
Figure 7: Comparison of $|u_h - u|$ for different values of $\sigma$. For a) $\max |u_h - u| = 0.03123$, for b) $\max |u_h - u| = 0.03389$, for c) $\max |u_h - u| = 0.2348$ and for d) $\max |u_h - u| = \infty$. The RHS is equal to $e^x \cdot e^t$. Here all colour maps appear as grey-scale.

(b), we observe that the $l_p$-error is smaller for $\sigma = 1$ when $p$ is large, e.g., $p = \infty$, while it is smaller for $\sigma = \sigma_0$ when $p$ is small, e.g., $1 \leq p \leq 2$. This observation is related with the fact that for $\sigma = 1$ the difference scheme is unconditionally stable in $l_\infty$ while for $\sigma < 1$ the stability depends on the ratio of $h^2$ and $\tau$ (see [8], Section 5.1.7). On the other hand, the difference scheme is unconditionally stable in $l_p$ for $p = 2$ for all $\sigma \in \left[\frac{1}{2}, 1\right]$ and is
stable for all $\sigma \in [\sigma_0, 1]$. Note that this range contains $\sigma = \frac{1}{2}$ where the
error in the $l_2$-norm is $O(h^2 + \tau^2)$ which is better than the error $O(h^2 + \tau)$
for $\sigma = 1$. Moreover, for $\sigma = \sigma^* \in [\sigma_0, \frac{1}{2}]$ (see also Section 1 and Section
4) the error rate may improve even to $O(h^4 + \tau^2)$.

• For the unstable cases (c) and (d) the black colour means that the absolute
error is out of the range given at the right-hand colour bar. Case (c) and
(d) show that, despite of the fact that the error is locally distributed
in a seemingly chaotic way, there is a very clear global pattern for this
distribution, as follows:

1. in the beginning of the process (i.e., for sufficiently small $t > 0$) the
approximation remains consistent (this corresponds to the blue-green
band (i.e., to small-to-medium absolute value in the colour (mode 1)
mapping) and the left-hand side of the domain in (c) and (d));
2. the length of this initial period depends on $x$ (it is shorter closer to
the ends $x = 0$ and $x = 1$, and longer in the middle of $[0, 1]$;
3. the length of this initial period depends crucially on $\sigma$ (it decreases
rapidly as $\sigma$ decreases from $\sigma_0$ to 0;
4. the ”blue” (”small absolute value of error”, in colour (mode 1) terms),
”red” (”large absolute value of error”) and ”black regions” (”absol-
ute value of error too large/out of range”) are fairly regular in shape
and depend crucially on the value of $\sigma \in [0, \sigma_0)$.

4. Concluding Remarks

Part of the material of this section has been announced in Section 4 of the
unpublished preprint [2].

The integral representation of the solution (4) in [3] is derived in Appendix
A.2 of [3] only for sufficiently smooth data (RHS, initial-values and boundary-
values) of the initial-/boundary-value problem, because this formula is obtained
from (5) in [3], which is valid only for sufficiently smooth data. In fact A.2 in
[3] can be appropriately extended for less regular, even distributional, data by
using a very general standard continuity/density argument which is described,
e.g., in [7], Chapter I, Theorem 7. The full analysis and technical details of this
standard argument will not be discussed explicitly here.
Let us note that it is possible to approximate consistently the solution (4) in [3] of the parabolic problem (2) in [3] also in the case of less regular RHS and initial and boundary conditions in (4) in [3], by using low-order quadratures with densely defined knot vector (as was done in [4]). We have not included visualization of such cases here, but we would like to add one important observation as a concluding remark to this case, as follows.

Assume that the solution (4) in [3] has singularities or changes smoothly but with very sharp spatial inhomogeneity (almost singularity), e.g., steep change of directional derivative, etc. Assume also that the step \( h \) and \( \tau \) are such that the difference scheme is stable for every \( \sigma \in [0,1] \), that is, \( \sigma_0 = \frac{1}{2} + \frac{h^2}{4\tau} \), or \( 0 < \tau \leq \frac{h^2}{2} \). Then, the singularities of the solution (4) in [3] are approximated best by the solution of the explicit scheme (17)-(19) in [3], i.e., for \( \sigma = 0 \). As \( \sigma \) increases from 0 to 1 (from "fully explicit" to "fully implicit" scheme), the approximation of the singularities deteriorates, in the sense that they get increasingly over smoothed (underfitted). Thus, when the solution of (4) in [3] is not very smooth, it is recommendable to use difference scheme (14) in [3] with \( \sigma = \sigma_0 \) (or \( \sigma > \sigma_0 \) but \( \sigma \) close to \( \sigma_0 \)). Thus, for problems with non-smooth RHS and/or initial/boundary data, we recommend to use small step in the time variable \( (0 < \tau \leq \frac{h^2}{2}) \) and explicit scheme (14) in [3], i.e., \( \sigma = 0 \), whenever possible. In this case the choice \( \sigma = 0 \) has also the obvious additional advantage that the matrix of the equations is triangular.

There is rich diversity of topics for further work on scientific visualization in the field of PDEs and their solutions. Here we give only one simple special topic and one advanced general topic, as follows.

- In the error visualization in Subsection 3, it is of considerable interest to study and visualize also the error distribution for the scheme with higher rate of local approximation \( O(h^4 + \tau^2) \) for \( \sigma = \sigma^* = \sigma_2^* = \frac{1}{2} \left(1 - \frac{h^2}{6\tau}\right) \) and special RHS in (17)-(19) in [3], where \( F_{ij} \) in (18) in [3] should be replaced by

\[
F_{ij} = \frac{5}{6} F_{ij} + \frac{1}{12} (F_{i-1,j} + F_{i+1,j})
\]

(see [8], Section 5.1.3).

- Of great interest is the visualization of the error distribution for iterative methods of approximate solution of non-linear ODEs and PDEs.

See also the concluding remarks in [3] and [5].
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