Travel–time calculation in heterogeneous 3-D structures *

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Summary

The selection of the numerical method to calculate travel times depends on the nature of the travel times, on the complexity and computer representation of the seismic model of the geologic structure, on the geometry of the set of points at which the travel time is to be calculated, and on the accuracy required. Various numerical methods, including the most recent ones, are discussed from the point of view of the travel–time calculations in general 3-D heterogeneous block structures with curved structural interfaces. The main attention is paid to the applicability and limitations of the methods, and to demonstration of their accuracy.

1 Introduction

The number of numerical methods to trace rays and calculate travel times is increasing and new, more accurate and reliable methods are emerging. On the other hand, these methods are being developed for different purposes, different seismic models of a geologic structure, and may calculate different kinds of travel times. Moreover, these methods are often incomplete: a method estimating rays and travel times with insufficient accuracy (like network shortest–path ray tracing) may be very valuable preprocessor requiring a postprocessing method (like bending) to increase accuracy, while some other methods like, for instance, bending, are only very powerful postprocessors requiring a preprocessing method to submit semi–finished rays and travel times. The results of such postprocessing methods are then dependent on their preprocessor, and the same method (e.g. same bending) may yield completely different travel times for different preprocessors. A complete algorithm to calculate travel time has then often be composed of several steps, each of them has commonly been referred to as an individual ray tracing method in the geophysical literature. This further increases the number of possible algorithms to calculate travel times.

Different methods of travel time calculation thus usually do not compete, especially if they are based on a sufficiently different principle. Only the algorithms within individual classes of methods may be mutually competitive, and are being developed towards a better accuracy, reliability, and efficiency.

One should thus supersede hesitating between different ray tracing methods by creating numerical modelling environment in such a way to enable application of a largest possible variety of ray, travel–time, and wavefield calculation methods, both present and future. A special attention should be paid to the possibility of a particular algorithm to estimate the accuracy of the calculated travel time. Even very accurate method is worthless if its accuracy in the model under consideration is unproved.

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This contribution is intended to briefly illustrate the differences between several methods to calculate travel times in complex heterogeneous 3-D structures, their accuracy, and applicability.

2 Selecting the travel–time calculation method

When selecting the travel–time calculation method, one should consider at least the following criteria:

(a) *Model specification:* The calculation algorithm must be conformal with the selected model specification, and the model specification should be selected in such a way to enable application of most methods! There is a variety of possible model specifications, for example smooth model, gridded smooth model, cell model; smooth interfaces, triangularized smooth interfaces, interfaces composed of triangles, etc. Some of these representations may be converted into other ones within required accuracy, whereas other conversions are not possible. It is thus advisable to select *primary model* specification in such a way to allow for conversion to the most other important model representations.

(b) *Type of travel time required by the application:* In particular, the *first arrival travel times* (often but not always required in seismic travel–time tomography) should strictly be distinguished from *elementary travel times* (necessary, for instance, in ray–theory based migrations).

(c) *Geometry and accuracy determined by the application:* Reasonably fast calculation of travel times on dense rectangular grids of points for migrations or hypocentre determinations may require different methods than very accurate two–point ray tracing between several sources and receivers.

3 Model

The model specification should be selected in such a way to be suitable not only for all possibly required contemporary travel–time calculation and wavefield modelling methods, but also to maximize the possibility of convenient application of unknown, future methods. After selecting the model parametrization, one should avoid to calculate travel times for different model, although described in terms of the same numerical values. For instance, gridded smooth models should never be confused with cell models, but sometimes may be substituted if the error of the substitution is correctly accounted for.

3.1 Physical meaning and computer representation of the model

Seismic model of the medium is, as a rule, specified by a finite set of values (model parameters), and of the rules or procedures expressing the dependence of spatial variations of material properties on these values. Since the exact material properties are fractal in the nature, the material properties described by the model are, as a rule, smoothed approximations of exact ones. Thus the *smoothness* is a natural property of a seismic model. Moreover, probably all contemporary numerical methods of wavefield or travel–time calculation require in some sense smooth models.

3.2 Continuous model representations

There are many kinds of continuous model representations. For instance, geological blocks may be described in terms of *volume modelling* (Gjøystdal, Reindhardsen & Åstebøl 1985, Červený, Klimeš & Pšenčík, 1988) or *surface modelling* (CAD–like) techniques, with structural interfaces and material parameters (like propagation velocities) represented by means of *explicit* and *implicit* or *parametric* representations of various degree of smoothness.

3.3 Grid representations of the model

For methods to calculate travel times (and also for methods to calculate complete wavefields) on a rectangular grid of points, the same grid slowness values may represent different models. The most important kinds of a seismic model represented in terms of grid values are a *cell model* composed of rectangular homogeneous cells, and *gridded smooth model* composed of discrete slowness values at gridpoints, corresponding to a smooth model. The *smooth model* may be a smooth model without interfaces, or a *smooth block model.* In the *smooth model without interfaces*, the slowness is a smooth function of spatial coordinates. The *smooth block model* is composed of blocks of arbitrary shapes separated by structural interfaces covered by a finite number of smooth surfaces. Inside each block, the slowness is a smooth function of spatial coordinates. Since the uncertainty of the interface position in a gridded smooth block model is of the order of grid step h, the gridded smooth block models should be supplemented by gridded block indices and by gridded information on the position of structural interfaces if a better travel–time accuracy than of the order h is required.

3.4 Dependence of travel times on model parametrization

Assume to replace gridded smooth model without interfaces by the cell model with the same grid slownesses. Then the relative differences of travel times corresponding a cell model and to a smooth model are of the order $h^{3/2}$ for turning rays (rays touching a coordinate plane), and of the order h^2 for rays nowhere parallel with any coordinate plane. Assume to replace gridded continuous model with smooth interfaces by the cell model with the same grid slownesses. Then the relative differences of travel times corresponding a cell model and to a continuous model are of the order h^1.

3.5 Primary model and its conversion to secondary model representations

Different model representations need not be mutually convertible, that may result in incompatibility of subsequent travel–time and wavefield modelling algorithms. One should thus carefully select his *primary model computer representation* in order to be able to convert it anytime to other model representations (*secondary model representations*) suitable for various computational algorithms.

4 Initial–value ray tracing

4.1 Numerical solution of ray–tracing equations

Numerical solution of ray–tracing equations is the most general method of initial–value ray tracing in continuously specified smooth block models, see, e.g. Červený *et al.* (1988). Both the model–specification software and ray–tracing code are available in ANSI Fortran 77.

4.2 Semianalytical methods

Analytical solutions of ray–tracing equations are limited to special classes of propagation velocity distribution and thus cannot be globally applied to realistic 3-D models, similarly like *quadratures of ray–tracing equations* available only in media of a high symmetry, like 1-D models.

On the other hand, heterogeneous 3-D structures may be decomposed into small cells of, for instance, tetrahedral shape (triangles in 2-D), in which the slowness or velocity distribution has an analytical form suitable for analytical ray tracing. The ray is then composed of analytically evaluated elements situated within individual cells. Since the model has to be sufficiently smooth to enable application of initial-value ray tracing to, e.g., two–point ray tracing by shooting, or to calculation of ray–theory or Gaussian beam synthetic seismograms, semianalytical methods are valuable especially if the corresponding semianalytical models are sufficiently smooth (Körnig 1995a, 1995b) or if they are sufficiently accurate approximation of smooth models, similarly like gridded models. Under these conditions, the semianalytical methods may be viewed as some sort of numerical solution of ray–tracing equations, with similar applications.

5 Shooting

Shooting method is based on application of some sort of initial–value ray tracing algorithm. The principal problem of two–point ray tracing in heterogeneous block models consists in a sufficiently accurate determination of boundaries between rays with different ray history, i.e. passing through different geological blocks, across different structural interfaces, or terminated in different areas for different reasons. The demarcation belts between the different ray histories, corresponding to numerical uncertainty of the boundaries, have to be kept reasonably narrow, because all two–point rays, situated inside the demarcation belts, may be lost (Bulant 1994). On the other hand, determination of a two–point ray within a single ray history is usually a trivial task, although more frequently addressed in geophysical literature than demarcating the ray histories.

6 Controlled initial–value ray tracing

Controlled initial–value ray tracing is closely related to shooting. Its aim is not to hit given receivers, but to cover the model with a sufficiently dense system of rays (or to cover the given surface with a sufficiently dense system of ray endpoints). That is why the demarcation of ray histories and the triangularization of take–off parameters of rays of the same history play the principal role in controlled initial–value ray tracing.

7 Wavefront tracing

In the wavefront tracing method, complete wavefronts are discretized with a sufficient density and traced along short ray elements from preceding to succeeding one, see Vinje, Iversen & Gjøystdal (1993) for 2-D and Vinje, Iversen, Gjøystdal & Åstebøl (1993, 1995) for 3-D. The density of rays is continuously adjusted by means of interpolation. This method is basically equivalent to controlled ray tracing, but the total length of traced rays may be about three times shorter in 3-D. On the other hand, the rays are traced by parts that corresponds to the difference between Runge–Kutta and Hamming's predictor–corrector methods and may slow down tracing, sometimes even more than twice (Červený *et al.* 1988). Thus the speed of wavefront tracing need not be much better than that of controlled ray tracing.

8 Bending

Bending is not a complete method of ray tracing, it requires a preliminary approximation of the ray estimated by means of another method. The accuracy of preliminary ray has to be sufficient in order to distinguish the required ray strictly from other extremal paths. Bending may be especially valuable to postprocess the results of network shortest–path ray tracing for the purposes of first–arrival travel–time tomography (Moser, Nolet & Snieder 1992). Bending is suitable for application in smooth models and, if properly coded and supplemented with a proper preliminary ray tracing algorithm, should be sufficiently accurate for any seismic application.

In a smooth models without interfaces, bending is relatively simple problem solvable using paraxial ray approximation (Farra 1992) iteratively, no systems of linear equations for ray points often used in the past are necessary. In smooth block models with structural interfaces, bending may lead to iterative linear programming, like for instance simplex method, or, especially for first arrivals, an iterative travel–time minimization by local ray perturbations based on Fermat's principle may be applied.

9 First-arrival travel–time calculation on a rectangular grid of points

In recent years, following the extension of random–access computer memory (RAM), many authors proposed the methods of calculating travel times on regular rectangular grids of points. The grids represent the discretized forms of seismic models, like in full–wave finite difference methods. As a rule, the grid travel–time calculating methods have been proposed for first–arrival travel times.

The accuracy of calculated travel–time depends on the grid step h — the distance between two neighbouring gridpoints. We refer the travel–time calculation or wavefield–modelling method to the method of the n^{th} order (order h^n) if the error of travel time is proportional to h^n for sufficiently small grid steps h. Because of memory limitations of present computers, the methods of the first or smaller orders do not usually meet the accuracy requirements of the contemporary geophysics in inhomogeneous 3-D structures.

9.1 Network shortest–path ray tracing

Network shortest–path ray tracing methods, based on Fermat's principle and the graph theory, are designed to calculate first–arrival travel times. They developed from the less accurate methods of the orders between 0 and ⅔ by Nakanishi & Yamaguchi (1986), Moser (1989, 1991), and Saito (1989, 1990), to the self–adaptable algorithm of the first order by Klimeš & Kvasnička (1994). The method is very reliable and the corresponding computer code is available in Fortran 77. On the other hand, the accuracy of the order h^1 (see Fig. 1) is not sufficient for 3-D travel–time tomography and the method should thus be supplemented with a bending method. Another disadvantage is the computation time increasing in 3-D with h^{-4}.

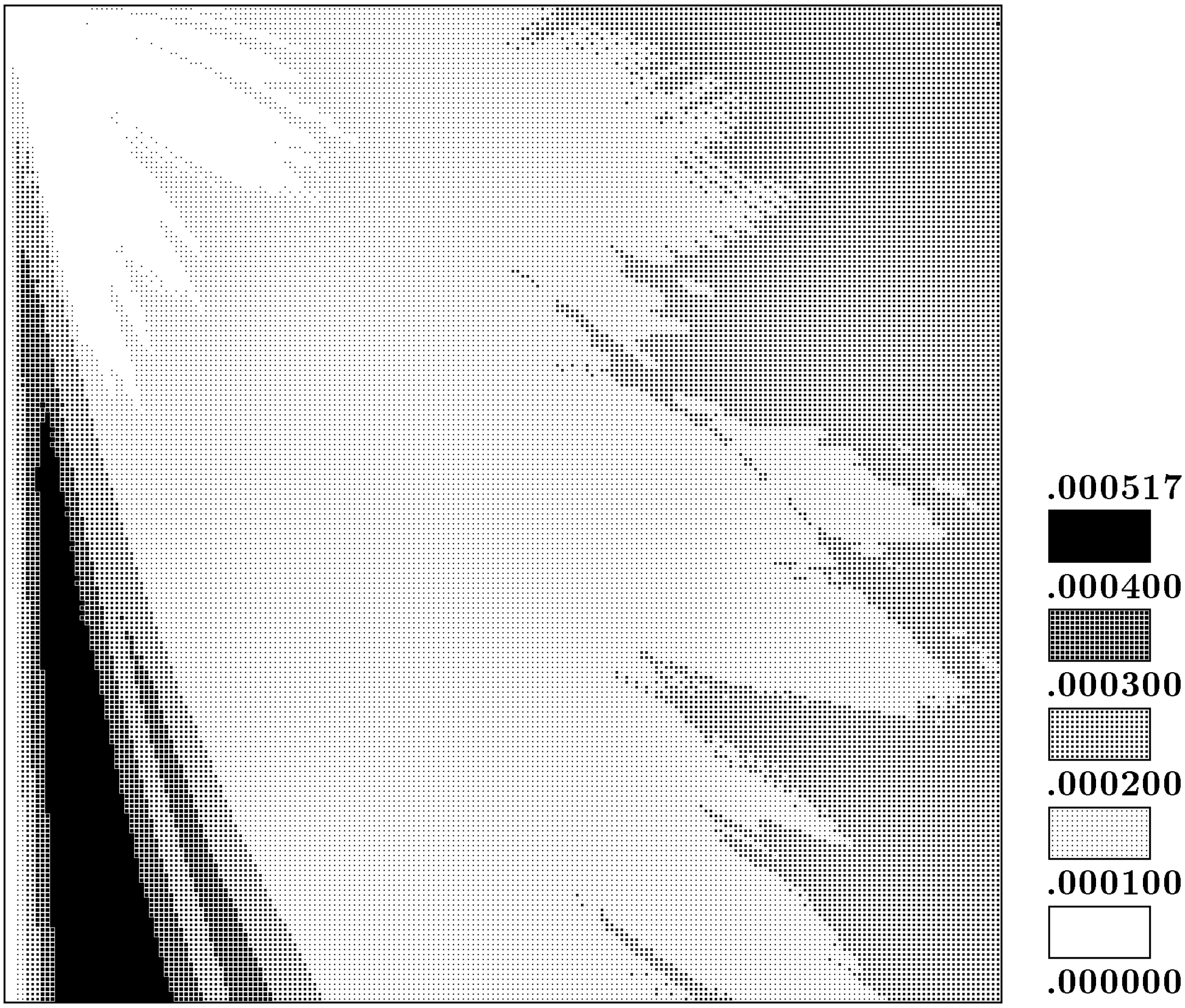

Figure 1. Travel–time errors of the network shortest–path ray tracing according to Klimeš & Kvasnička (1994) in a constant velocity gradient model (velocity increases linearly with depth, the velocity ratio between top and bottom is 1:3, the source is situated at the left–hand top corner of a vertical square in which the travel times are calculated). In this model, the first–arrival travel times coincide with elementary travel times. The absolute errors of the travel time are scaled in seconds. Program `NET` version `2.00`. Let us note that the errors of the first–order grid travel–time tracing method by Podvin & Lecomte (1991) are roughly twice greater, see Klimeš, Kvasnička & Červený (1994).

9.2 Grid travel–time tracing of the first order

Under *grid travel–time tracing* we understand here the methods interpolating already calculated travel times between gridpoints in order to evaluate the travel time in the closest next gridpoint. These methods are often called "finite–difference" eikonal–equation solvers, but the ordinary meaning of "finite–differences" would have to be generalized considerably to include also these methods. These methods developed from the non–causal (and thus practically unusable) idea of Vidale (1988) to the stable method of the first order by Podvin & Lecomte (1991). The computation time of their algorithm should increase in 3-D with h^{-3}, but the accuracy of the order h^1 (approximately twice worse than of the above network shortest–path ray tracing, see Klimeš 1995) disables its application to 3-D travel–time tomography without postprocessing like a bending method.

9.3 Grid travel–time tracing of the second order

The accuracy of the grid travel–time tracing methods may considerably be increased by replacing the plane wavefront approximation by a method of higher order, if the updating scheme is made stable for the interpolation method.

A very reliable method of the second–order accuracy applicable to general 2-D and 3-D *cell models* has been proposed by Ditmar (1995). To enable quadratic interpolation of travel times, the method calculates travel times, in addition to gridpoints at the corners of cells, also in additional points situated at the gridlines in the middle between the pairs of neighbouring gridpoints. Thus the number of calculated travel times is four times the number of gridpoints in 3-D. Since designed for cell models, the algorithm is not applicable to gridded smooth models, especially to models with smooth interfaces, without a considerable loss of accuracy.

The method proposed by Klimeš (1995) for *gridded smooth models* is based on the idea of calculating the slowness vectors at gridpoints together with travel times. The travel times between two adjacent gridpoints are interpolated by a second–order or third–order method. The point on the gridline segment, from which the ray propagates to the next gridpoint, is approximated with the accuracy proportional to the squared grid step. The linear interpolation is used for the slowness. From the point on the gridline segment, the slowness vectors and travel times are approximated by expansions accurate up to terms with second partial travel–time derivatives. Thus, in a smooth media, the resulting travel–time error corresponds to the neglected second partial slowness derivatives, and is of the order of the squared grid step. Then the rays are approximated very accurately in smooth parts of a model, i.e. in the regions where the second partial slowness derivatives are kept within some reasonable finite limits. The algorithm of the accuracy order h^2 (see Fig. 2) is designed for a smooth model without the first and second order interfaces, but it probably may be generalized for smooth block models using travel–time matching at structural interfaces. Computer costs are of the order h^{-3}. This method is thus very promising for first–arrival travel–time tomography, but there is no computer code available these days .

10 Calculating elementary travel–times at gridpoints of a rectangular grid

Some seismic applications, like ray–theory based migration techniques or nonlinear determination of seismic hypocentres, require the elementary travel times corresponding to most energetic arrivals to be known at a large number of gridpoints of a sufficiently dense 3-D rectangular grid of points. The density of the grid should, if possible, enable to interpolate multivalued travel times between gridpoints, in order to adjust the grid density for a particular application and frequency band.

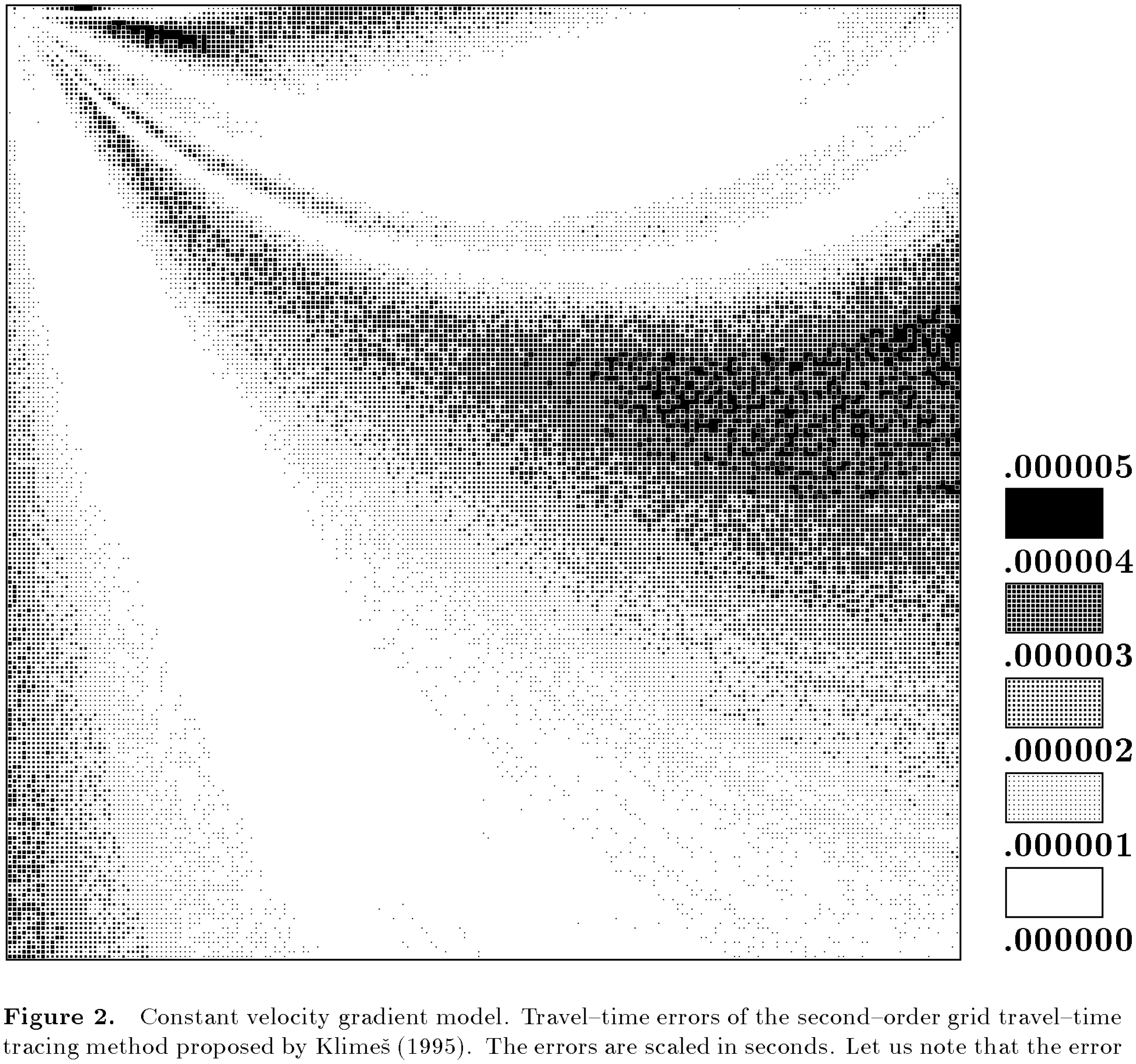

Figure 2. Constant velocity gradient model. Travel–time errors of the second–order grid travel–time tracing method proposed by Klimeš (1995). The errors are scaled in seconds. Let us note that the error distribution has somewhat random nature since the rounding errors are of the order of 0.000001 s before subtracting. Moreover, the numerical errors of evaluating analytical travel times may reach at some points absolute error of 0.000002 s or even more. For example, the error at the second gridpoint of the top row in Figure 3b is due to the analytical solution, grid travel–time tracing is much more accurate there. Program `TTT-2D` version `0.06`.

10.1 Weighting of paraxial ray approximations

Initial–value ray tracing may yield the points along all traced rays, stored with a given step. Unfortunately, the points are distributed irregularly in space and the travel times are multivalued that prevents application of routine interpolation techniques. If the system of rays is sufficiently dense and the step along rays is reasonable, the travel times and all other calculated quantities may be interpolated by weighting paraxial ray approximations. The method has been proposed by Klimeš (1994) for nonlinear hypocentre determination, and its accuracy and applicability has been demonstrated by Klimeš, Kvasnička & Červený (1994), see Fig. 3.

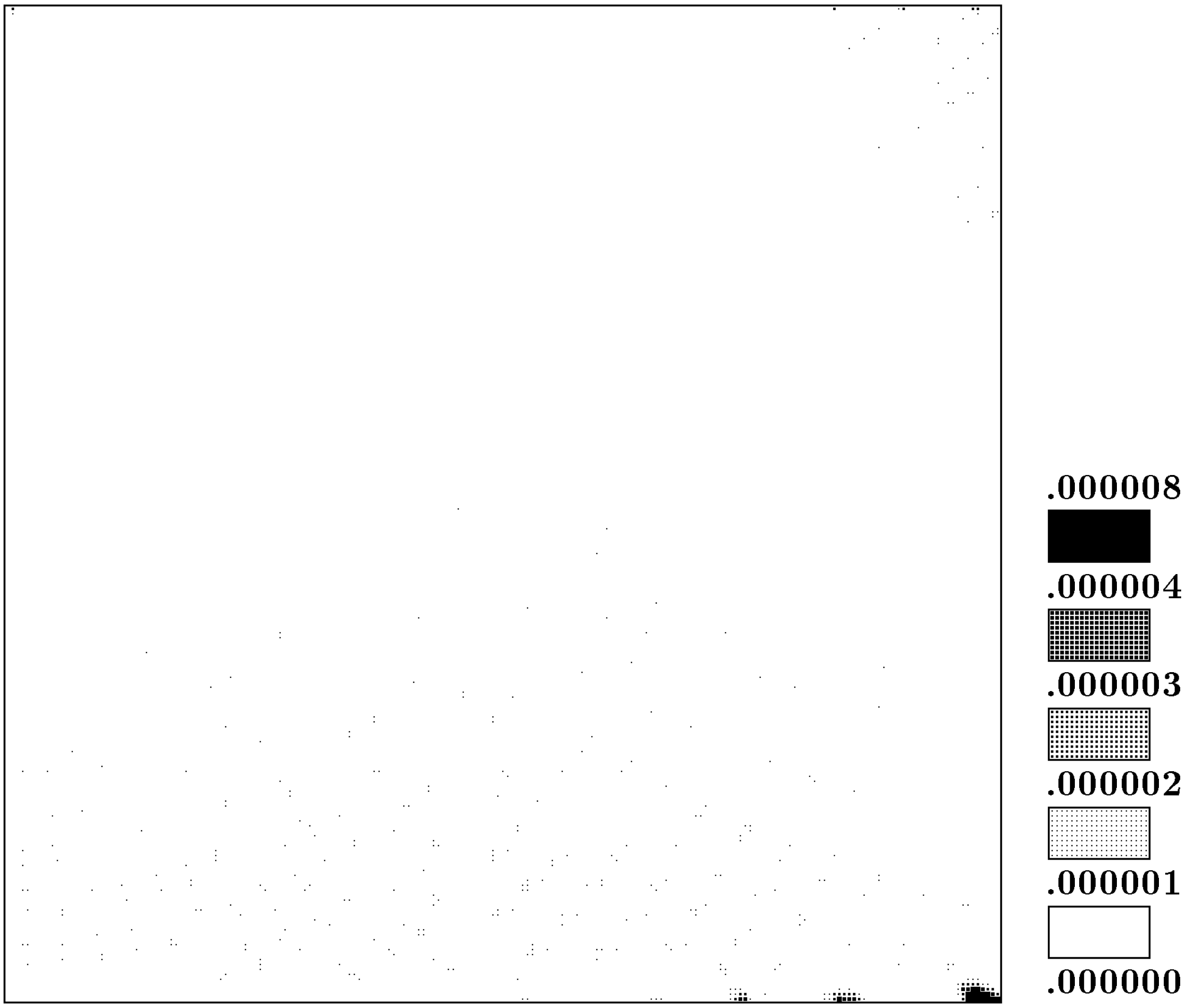

Figure 3. Constant velocity gradient model. Travel–time errors corresponding to weighting of paraxial ray approximations proposed by Klimeš, Kvasnička & Červený (1994). The errors are scaled in seconds. The initial–value rays were shot with the angular step of $1.125°$, and points along the rays were stored with the step of 0.0175 s. Let us note that, as in Fig. 2, the error distribution has somewhat random character since the rounding errors are of the order of 0.000001 s, and the numerical accuracy of evaluating the reference analytical travel times is, at some gridpoints, even worse. Program `INTER` version `0.30` with default numerical parameters.

Since the initial–value ray tracing itself is not capable to guarantee a sufficient coverage of the target zone, in which the grid is situated, by rays, this method is unsafe unless *controlled initial–value ray tracing* or *wavefront tracing* is used.

10.2 Interpolation of the results of wavefront tracing or controlled initial-value ray tracing

In controlled initial–value ray tracing and wavefront tracing, the 2-D space of ray take–off parameters is, as a rule, triangularized or may well be decomposed to 2-D cells of another shape. In this way the space between two consecutive wavefronts is decomposed into 3-D ray cells. If this information is available during interpolation process and the location of gridpoints with respect to ray cells is ascertainable, travel times and all other calculated quantities may routinely be interpolated within individual ray cells. Unlike weighting of paraxial ray approximations, this method is capable to strictly comply with the boundaries of shadow zones.

11 Conclusions

Primary model computer representation should be carefully selected to enable modelling of sufficiently general heterogeneous 3-D geological structures, to provide sufficient smoothness for most of travel–time and wavefield modelling methods, and to allow for sufficiently accurate and reasonably simple conversion to *secondary model representations* covering the most important model representations and suitable for various computational algorithms, both present and future.

Grid travel–time tracing methods of the second or higher orders are the most promising methods to calculate *first-arrival travel–times.* Wavefront tracing could be modified for first arrivals, too.

For *first–arrival two–point ray tracing* network shortest path method supplemented with bending might also be used in addition of the above methods.

Wavefront tracing or controlled initial–value ray tracing complemented with several steps of consecutive interpolation seem now to be the best methods of calculating *elementary travel–times at gridpoints of a rectangular grid.* Grid travel–time tracing methods of the second or higher order also might contingently be generalized to elementary travel times in the future.

Shooting methods are suitable for *elementary travel–time two–point ray tracing.*

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