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Presentation of a gentle discretisation scheme for the numerical treatment of nonlinear heat conduction on unstructured grids in finite volume technique

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1. Introduction

For the numerical simulation of crystal growth equipment it is desirable to take nonlinear heat conduction into account, since the heat conductivity of nearly all materials shows a non trivial temperature dependence. Also in the modelling of heat transfer in semi-transparent media, which has a wide range of application, see e.g. Siegel and Howell (1972) or Vizman *et al.* (1996), effective conductivities $\sim T^3$ appear and have to be simulated. To have all the possibilities of local grid refinement in regions of special interest, unstructured grids are handled.

2. Unstructured grids

The grid treated here consists of a set of triangles. To discretise the governing partial differential equations in the finite volume manner several different strategies could be used.

In the:

- **cell storing method** the triangles serve as control volumes, while the values of the considered fields are stored in the centre of the triangle.

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- **vertex storing method** the values of the fields are stored in the vertices of the triangles. Each point is surrounded by a control volume, which can be constructed in several ways. You can follow the line from the middle point of an edge:
  - perpendicular to the edge till reaching the middle point of the surrounding circle. The correlated structure is the so called **Voronoi Diagram**;
  - to the centre of mass. The correlated structure is called a **Donald Diagram**. (We apply the terminology of Angermann (1995).)

In the following discussions the vertex stored method with associated Donald Diagram will be used (see Figure 1) because it provides a lot of advantages:

- The case of several materials $\lambda(x)$ does not possess any problems, since the fraction of the surface of the control volume in one triangle is embedded in one material with well defined conductivity.
- A simple treatment of boundary conditions is possible, e.g. Dirichlet conditions, the values stored on the boundary vertices are fixed and have not to be recalculated. They enter the equations just as constants.
- The control volume for a vertex in mind is restricted to those triangles which are surrounding this vertex, even in the case for angles > 90°.
- The expansion of 1D discussions to more dimensions is obvious.

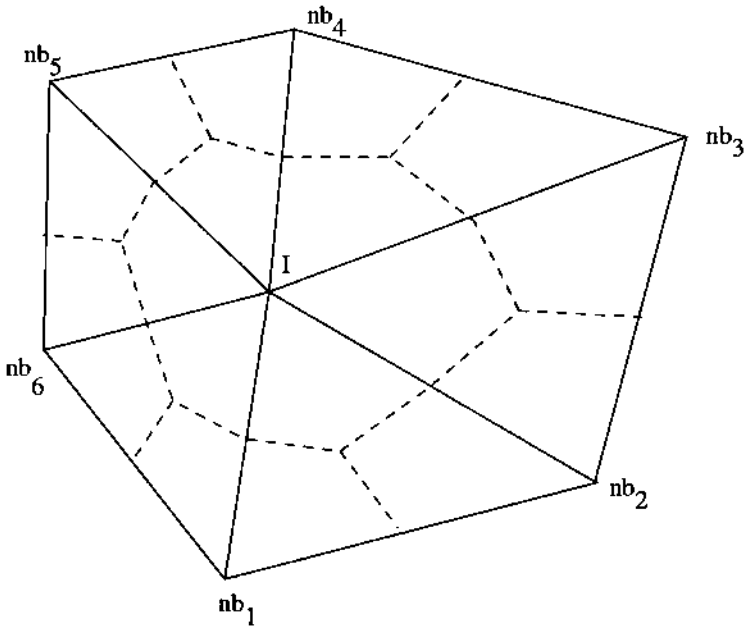

Figure 1. Excerpt of a 2D triangular grid with associated Donald diagram

Of course there are also disadvantages:

- The number of neighbours is not fixed.
- The corresponding discretised equations have no regular structure.

The above mentioned disadvantages have already been resolved: Dongarra *et al.* (1996) provide computational libraries in C++ including sparse matrix formats and also fully templated iterative solution procedures which were used to solve the appearing linear equations throughout this work.

3. Numerical treatment of heat transfer

3.1 Heat transfer by nonlinear conduction

In this section a proper discretisation scheme for the treatment of nonlinear heat conduction will be presented. This is done by showing the concerned problems in the 1D case. Some usually used discretisations are understood as approximations to the here presented one. Then the results are expanded to a 2D unstructured triangular grid.

Starting point for our discussion is the basic equation for heat conduction:

$$\frac{\partial}{\partial t} c_p \rho\, T + \operatorname{div} \vec{j}_T - s_T = 0 \tag{1}$$

where the heat current $\vec{j}_T$ is determined by Fourier's law.

$$\vec{j}_T = -\lambda(T)\, \vec{\nabla} T \tag{2}$$

As usual c_p labels the mass specific heat, ρ the density, $\lambda(T)$ the temperature dependent conductivity of the material and s_T the density of heat sources.

3.1.1 Discussion in one dimension

In the 1D, stationary case equation simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(-\lambda(T)\, \frac{\mathrm{d}}{\mathrm{d}x} T \right) - s_T = 0. \tag{3}$$

On the x-axis the vertex I may be surrounded by its neighbours L, R on the left and on the right side respectively. See Figure 2. After integration of equation (3) over the appropriate control volume (from l to r) we obtain the equation

$$\int_l^r \frac{\mathrm{d}}{\mathrm{d}x}\left(-\lambda(T)\, \frac{\mathrm{d}}{\mathrm{d}x} T \right) \mathrm{d}x - \int_l^r s_T \, \mathrm{d}x = 0.$$

The integral over the total derivative is performed. The source term approximated as usual:

$$-\lambda(T)\,\frac{\mathrm{d}}{\mathrm{d}x}T\Big|_r + \lambda(T)\,\frac{\mathrm{d}}{\mathrm{d}x}T\Big|_l - \Delta x\; s_T\Big|_I = 0 \tag{4}$$

Now, the task is to find an expression for the heat current on the surface of the control volume, that means in l, r respectively.

Therefore we consider equation (3) without sources, or equivalent

$$-\lambda(T)\,\frac{\mathrm{d}}{\mathrm{d}x}T = c. \tag{5}$$

The interpretation of the upper equation is trivial: the heat current is a constant in the absence of heat sources.

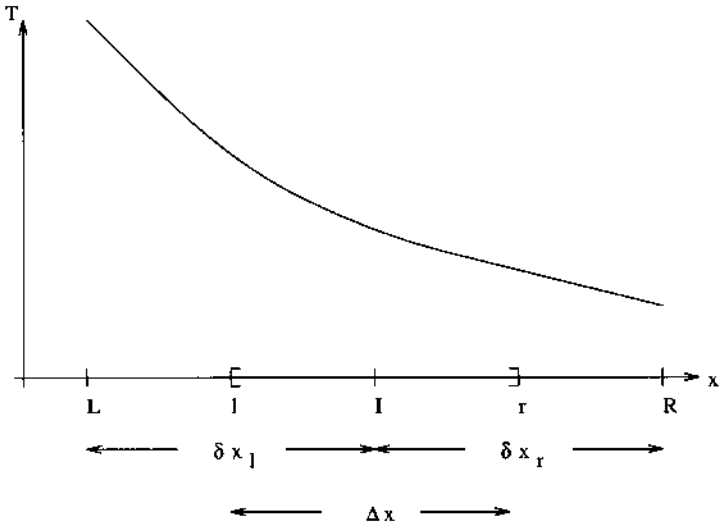

Figure 2. Vertex I with neighbours L and R and control volume (*l*, *r*)

At this point a very important statement can be given: the heat current is more smooth than the temperature field. If e.g. $\lambda(T)$ is discontinuous at an arbitrary temperature T_d, the temperature profile has a kink of that extension that the discontinuity of $\lambda(T)$ is absorbed, so that the current is constant all over the considered region.

We are interested in fixing the value c of the heat current by solving the boundary problem in any interval, e.g.

$$x \in [x_L,\ x_I]$$

with Dirichlet conditions

$$T(x_L) = T_L; \quad T(x_I) = T_I.$$

For further details see also Figure 2.

The parameterisation of the inspected interval

$$x = x_L + \gamma\,(x_I - x_L); \quad \gamma \in [0,1] \tag{6}$$

leads to the form

$$-\lambda(T)\,\frac{\mathrm{d}}{\mathrm{d}\gamma}T = \delta x_l\, c. \tag{7}$$

This differential equation can easily be solved by separation of variables.

$$-\int_{T_L}^{T_\gamma} \lambda(T)\,\mathrm{d}T = \int_0^\gamma \delta x_l\, c\,\mathrm{d}\gamma'$$

An integration over the whole interval finally yields

$$\int_{T_I}^{T_L} \lambda(T)\,\mathrm{d}T = \delta x_l\, c. \tag{8}$$

Because of the positivity of the heat conductivity

$$\lambda(T) > 0 \quad \forall\, T$$

the heat current increases (decreases) are strictly monotonic with T_L (T_I):

$$\delta x_l\,\frac{\mathrm{d}c}{\mathrm{d}T_L} = \lambda(T_L), \quad \delta x_l\,\frac{\mathrm{d}c}{\mathrm{d}T_I} = -\lambda(T_I) \tag{9}$$

Thus equation (8) is a one to one relationship between the heat current c and the temperatures T_L, T_I. Since this term holds over the whole interval we have found a proper expression for the left terms in equation (4). When the upper expression is used for fixing the current at the surface of the control volume we may call the resulting discretisation gentle, because it uses the smooth current and is soft to nonlinearities.

By doing approximations to the integral (8), one can achieve several simpler relations for the current in the surface point I of the control volume, which may be sited in the centre of the interval $[x_L, x_I]$:

- The central node approximation leads to the term you get, if you take the derivative $\frac{\mathrm{d}}{\mathrm{d}x}T$ to be a constant over the interval of interest and evaluate the heat conductivity at the temperature you get on the surface of the control volume by the same linear interpolation.

$$\delta x_l \, c_1 := \lambda \left(\frac{T_L + T_I}{2} \right) (T_L - T_I)$$

- Evaluation of the integral by the trapeze rule leads to a discretisation where the heat conductivity in *l* is guessed by the mean of the conductivities at both sides.

$$\delta x_l \, c_2 := \frac{1}{2} \Big(\lambda(T_L) + \lambda(T_I) \Big) (T_L - T_I)$$

- Harmonic interpolation, which is examined in the book of Patankar (1980) for the case of two materials with different heat conductivity touching each other at the surface of adjacent control volumes, leads to the form

$$\delta x_l \, c_3 := \frac{1}{2} \frac{\lambda(T_L)\lambda(T_I)}{\lambda(T_L) + \lambda(T_I)} \, (T_L - T_I).$$

It occurs that the physical properties (9) of the flux (since the measure of the surface (a point) is 1, heat current and heat flux are used synonymously) as a function of the temperatures at the boundaries are not necessarily conserved in these approximations. Figure 3 shows such a case. There the temperature in I has been fixed to T_I = 500K. A heat conductivity with an exponential dependence

$$\lambda(T) = \lambda_c \, e^{-\beta T}; \quad \beta = 0.001 \, K^{-1} \tag{10}$$

has been inserted (the change by a factor 2-4 in the range of 1,000 K is a typical temperature dependence for a lot of materials).

The heat flux is plotted as a function of the temperature T_I. Most of the schemes show the right behaviour if the difference between T_L and T_I is not

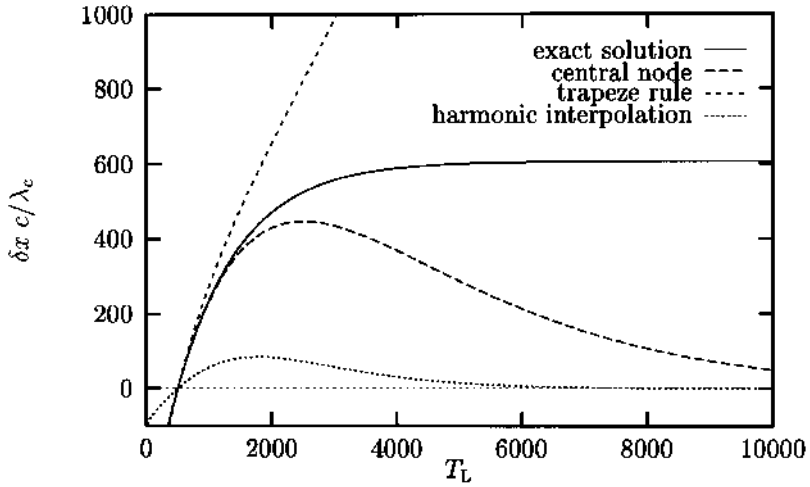

Figure 3. Flux for $\lambda(T) = \lambda c \, e^{-0.010K^{-1}T}$, T_I = 500K

great, but especially in the case for the central node approximation c_1 and the harmonic interpolation c_3 the estimated flux decreases with increasing temperature. This behaviour is quite unphysical. The solution T_L for a given flux becomes ambiguous, while that for the exact solution is unique. The trapeze evaluation c_2 does not show that phenomenon.

Since fluxes are equalised in the finite volume technique, these ambiguities are omnipresent. The behaviour of the approximated flux in the discretisation scheme may result in an unpredictable (oscillations, divergence, convergence to a wrong solution) behaviour of the iterative technique for the solution of the nonlinear equations – e.g. the Newtonian Solver – if the initial guess is not good enough, while it converges to the unique solution in the case of gentle discretisation, with which we want to proceed (the Newton method for multidimensional systems is explained in standard literature, e.g. Schwetlick (1979)).

By inserting (8) and its equivalent for the interval $[x_I, x_R]$ in (4), we obtain the governing equation for T_I.

$$\frac{1}{\delta x_l}\int_{T_L}^{T_I}\lambda(T)\,\mathrm{d}T+\frac{1}{\delta x_r}\int_{T_R}^{T_I}\lambda(T)\,\mathrm{d}T-\Delta x\; s_T\Big|_I=0. \tag{11}$$

This flux balance has to be done for every point which has to be calculated. In this manner we achieve a set of nonlinear equations. In most cases you will have no chance to resolve these relations analytically even in the case of one unknown temperature. But this formulation is perfectly suited for the Newtonian solver, because of the monotony of the appearing integrals.

Relation (11) leads to the following line in the matrix of the iterative scheme:

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \ddots \\ \cdots & -\frac{1}{\delta x_l}\lambda(T_L) & \left(\frac{1}{\delta x_l}+\frac{1}{\delta x_r}\right)\lambda(T_I) & -\frac{1}{\delta x_r}\lambda(T_R) & \cdots \\ \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \delta \begin{pmatrix} \vdots \\ T_L \\ T_I \\ T_R \\ \vdots \end{pmatrix} =$$

$$- \begin{pmatrix} \vdots \\ \frac{1}{\delta x_l}\int_{T_L}^{T_I}\lambda(T)\,\mathrm{d}T+\frac{1}{\delta x_r}\int_{T_R}^{T_I}\lambda(T)\,\mathrm{d}T-\Delta x\; s_T\Big|_I \\ \vdots \end{pmatrix} \tag{12}$$

In most relevant cases it may be sufficient to take $\lambda(T)$ in the iteration matrix and to approximate the integral at the right hand side by a Gaussian integration with three nodes, which is exact for polynomials up to 5th order.

$$\int_{T_1}^{T_0} \lambda(T)\,\mathrm{d}T \approx (T_0 - T_1) * \tilde{\lambda}$$

$$\begin{aligned}\tilde{\lambda} &= \frac{5}{18}\,\lambda\left(\frac{1+\sqrt{3/5}}{2}T_0 + \frac{1-\sqrt{3/5}}{2}T_1\right)\\ &+ \frac{8}{18}\,\lambda\left(\frac{1}{2}T_0 + \frac{1}{2}T_1\right)\\ &+ \frac{5}{18}\,\lambda\left(\frac{1-\sqrt{3/5}}{2}T_0 + \frac{1+\sqrt{3/5}}{2}T_1\right)\end{aligned}$$

To summarise the advantages of the gentle discretisation:

- The physical behaviour of the flux is fully respected.
- The set of discrete equations obtained by the discretisation does not become artificial ambiguous.
- The problem is smoothed for the Newtonian iterative solver, since only $\lambda(T)$ and $\int\lambda(T)\,\mathrm{d}T$ are needed, while in all other cases you must have the knowledge of $\lambda(T)$ and $\frac{\mathrm{d}}{\mathrm{d}T}\lambda(T)$ which could be a problem especially in the case of $\lambda(T)$ discontinuous or given as a table.

3.1.2 Expansion for two dimensions

Equation (1) is integrated over the control volume V_I surrounding vertex I, while divergences are transferred via the Gaussian Theorem into integrals over the appropriate surface.

$$\frac{\partial}{\partial t}\int_{V_I} c_p\rho\, T\,\mathrm{d}V + \oint_{\partial V_I} -\lambda(T)\,\vec{\nabla}T\,\mathrm{d}\vec{\sigma} - \int_{V_I} s_T\,\mathrm{d}V = 0 \qquad (13)$$

The surface integral may be split into its distributions from the several participating triangles.

$$\oint_{\partial V_I} -\lambda(T)\,\vec{\nabla}T\,\mathrm{d}\vec{\sigma} = \sum_{\Delta}\int_{\partial V_I|_\Delta} -\lambda(T)\,\vec{\nabla}T\,\mathrm{d}\vec{\sigma}$$

The further discretisation is done by applying the projection technique developed and investigated by Angermann (1995) for an upwind technique in the convective-diffusive case. Starting procedure is the approximation of the heat current by a constant vector $\vec{c}$ in the inspected triangle, which is an analogy to equation (5). (In the 1D case a constant heat current is the exact solution of the stationary problem without sources since there only the constant has no divergence. In the 2D case taking the heat current as a constant is a real approximation since you may find an infinite set of functions which have no divergence.)

$$-\lambda(T)\ \vec{\nabla}T = \vec{c} \tag{14}$$

We proceed by projecting this equation on one direction, e.g. edge $\overrightarrow{\mathrm{IR}}$. For unknown labels, see Figure 4.

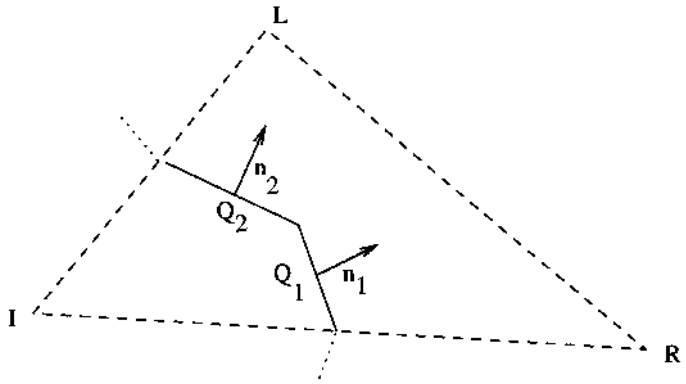

Figure 4.
A triangle with associated control volume

$$-\lambda(T)\ \vec{\nabla}T\ \vec{\mathrm{IR}} = \vec{c}\,\vec{\mathrm{IR}}$$

A parameterisation of the edge is used as in (6).

$$\vec{x} = \vec{\mathrm{I}} + \gamma\,\vec{\mathrm{IR}} \quad \gamma \in [0,1]$$

Application of the chain rule leads to the analogy of (7):

$$-\lambda(T)\ \frac{\mathrm{d}}{\mathrm{d}\gamma}T = \vec{c}\,\vec{\mathrm{IR}}$$

The integral is performed in order to get the heat current in the $\overrightarrow{\mathrm{IR}}$ direction.

$$\vec{c}\,\vec{\mathrm{IR}} = \int_{T_{\mathrm{R}}}^{T_{\mathrm{I}}} \lambda(T)\,\mathrm{d}T$$

The same treatment leads to the expression for the projection in $\vec{\mathrm{IL}}$ direction.

$$\vec{c}\,\vec{\mathrm{IR}} = \int_{T_\mathrm{R}}^{T_\mathrm{I}} \lambda(T)\,\mathrm{d}T$$

For the projection of the heat current in either the $\vec{\mathrm{IR}}$ or $\vec{\mathrm{IL}}$ direction the discussion of the 1D case may be applied.

We expand the vector $\vec{c}$ in the coordinates $\vec{\mathrm{IR}}_\perp$, $\vec{\mathrm{IL}}_\perp$

$$\vec{c} = (2A_\Delta)^{-1}\left((\vec{c}\,\vec{\mathrm{IL}})\,\vec{\mathrm{IR}}_\perp - (\vec{c}\,\vec{\mathrm{IR}})\,\vec{\mathrm{IL}}_\perp\right)$$

and finally obtain the desired expression for the flux through the surface of the control volume of the point I in the treated triangle (this is the expression one obtained in the 3D rotational invariant case. To get the real 2D equations set $(\mathrm{Q_1})_r = (\mathrm{Q_2})_r = 1$).

$$12A_\Delta \int_{S_\Delta} -\lambda(T)\,\vec{\nabla}T\,\mathrm{d}\vec{\sigma} \cong$$

$$+\left((\mathrm{Q_1})_r\,(\vec{\mathrm{LI}} + \vec{\mathrm{LR}})\,\vec{\mathrm{IR}} + (\mathrm{Q_2})_r\,(\vec{\mathrm{IR}} + \vec{\mathrm{LR}})\,\vec{\mathrm{IR}}\right)\int_{T_\mathrm{L}}^{T_\mathrm{I}} \lambda(T)\,\mathrm{d}T$$

$$-\left((\mathrm{Q_1})_r\,(\vec{\mathrm{LI}} + \vec{\mathrm{LR}})\,\vec{\mathrm{IL}} + (\mathrm{Q_2})_r\,(\vec{\mathrm{IR}} + \vec{\mathrm{LR}})\,\vec{\mathrm{IL}}\right)\int_{T_\mathrm{R}}^{T_\mathrm{I}} \lambda(T)\,\mathrm{d}T$$

where we have employed the notation of Figure 4.

The following expressions have been used:

$$\vec{n}_1 = \frac{1}{6}\,(\mathrm{Q_1})_r\,(\vec{\mathrm{LI}} + \vec{\mathrm{LR}})_\perp$$

$$\vec{n}_2 = \frac{1}{6}\,(\mathrm{Q_2})_r\,(\vec{\mathrm{IR}} + \vec{\mathrm{LR}})_\perp$$

$$(\mathrm{Q_1})_r = \frac{1}{12}(5\mathrm{I}_r + 5\mathrm{R}_r + 2\mathrm{L}_r)$$

$$(\mathrm{Q_2})_r = \frac{1}{12}(5\mathrm{I}_r + 2\mathrm{R}_r + 5\mathrm{L}_r)$$

The index r indicates the radial coordinate of a vector.

3.1.3 Another point of view

After the upper treatment of nonlinear conduction, the procedure shall once more be justified.

If we define an antiderivative $\Lambda(T)$ of the heat dependent conductivity $\lambda(T)$

$$\frac{\mathrm{d}}{\mathrm{d}T}\,\Lambda(T) = \lambda(T),$$

then by application of the chain rule we are able to rewrite Fourier's law (2):

$$\vec{j}_T = -\vec{\nabla}\Lambda$$

Thus Λ is a potential for the heat current. In terms of this potential the stationary problem is linear.

$$\mathrm{div}\,\vec{\nabla}\Lambda - s_T = 0 \tag{15}$$

This strategy is sometimes called Kirchoff transformation. For the discretisation of equation (15) the potential Λ can without danger be interpolated in a linear manner. Thus $\vec{\nabla}\,\Lambda$ is taken as constant on the numerical entity. At this point it shall be emphasised that the heat current is approximated as a constant and not the gradient of the temperature field. This treatment is obviously equivalent to the upper presented one. But the projection technique has a grater range of application. It may also be used – as already mentioned – to solve the convective-diffusive problem for heat transfer in fluid mechanics.

3.1.4 Test case

The test case consists of a cylinder with length δx and radius δx. The heat conductivity is taken as in the 1D example (10). The cylinder walls are treated adiabatically, while the temperatures at the bottom T_{bot} and the top T_{top} are fixed to

$$T_{\mathrm{bot}} = 500K; \quad T_{\mathrm{top}} = 10000K$$

in the first case and to

$$T_{\mathrm{bot}} = 500K; \quad T_{\mathrm{top}} = 2000K$$

in the second.

We are able to write down an analytic expression for the temperature profile.

$$T(x) = -\frac{1}{\beta}\,\ln\left(\left(1 - \frac{x}{\delta x}\right)e^{-\beta\,T_{\mathrm{bot}}} + \left(\frac{x}{\delta x}\right)e^{-\beta\,T_{\mathrm{top}}}\right)$$

The initial guess for the iterative solver is a constant temperature profile for all points which have to be calculated.

$$T_{\text{init}} = 500K$$

In the first example we are in the interesting range, where the other discretisation schemes should run into problems with the wrong slope of the flux. This is reflected in the solution as you can easily see in Figure 5. There the exact temperature profile is compared with the calculated temperatures at the symmetry axis of the cylinder. Only the central node and the gentle scheme are compared, since after that the two other schemes provide no astonishment. The solver converged to a wrong solution of the ambiguous discrete equations. In the second example, Figure 6, the central node scheme is tested to be well implemented for a temperature out of the critical range. The calculations for both cases were performed on the grid shown in Figure 7. It consists of 439 vertices. We used the grid generator N2 (Eichenseher, 1996) developed at the Institute for Applied Mathematics, Technical University of Munich.

The next question is, of course, the grid dependence of the statements; only the central node scheme is of further interest. Therefore the stated problem was solved on two more grids with 2,673 and 10,535 vertices respectively. The initial guess for the start solution is unchanged, so the statement that the central node scheme should run into trouble stays true in all grids, since – at least in the first iterative step – the temperature difference is the same in vertices near to the boundaries; only the distance has been changed. The result is plotted in Figure 8. We immediately see, that grid refinement is no panacea. Though with grid refinement the error may decrease in the L^2-sense, an engineer who is interested in the L^∞-error will state an increasing error.

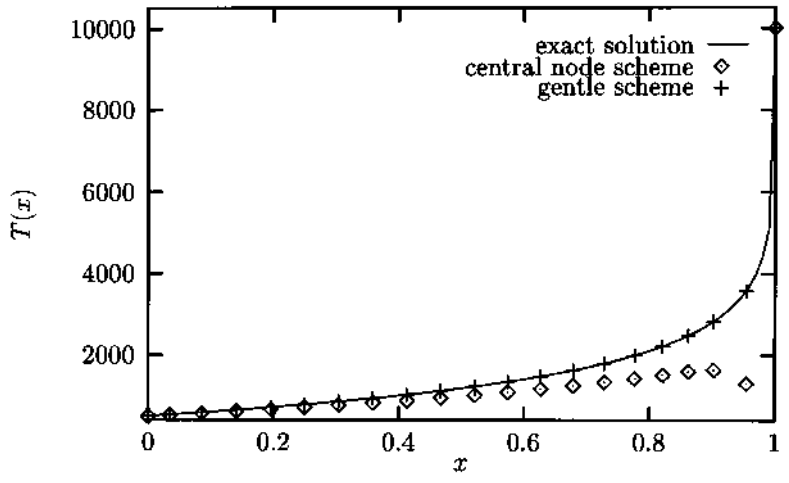

Figure 5.
Comparison of the exact solution of two possible discretisations

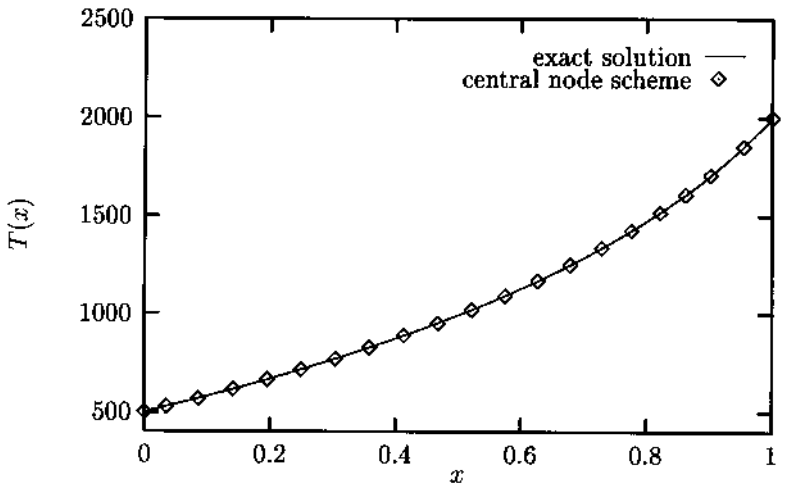

Figure 6.
Proof for the correct implementation of the central node scheme

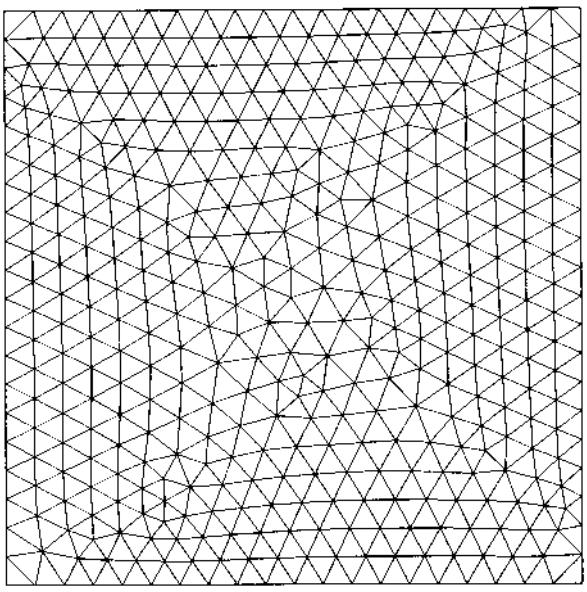

Figure 7.
Grid for test calculation

3.2 Boundary conditions

To be exact in the mathematical sense, it is not enough to examine the equation for heat conduction (1). For the problem to be well defined, a region G has to be specified in which the equation has to be solved, as well as boundary conditions on the border ∂G of G (see Figure 9). When needed, $\vec{\nu}$ labels the outer normal vector of ∂G.

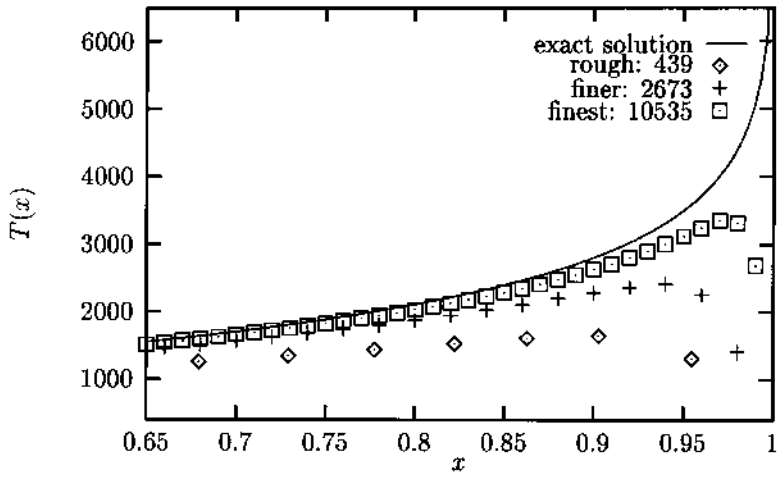

Figure 8. Grid dependence of the central node scheme

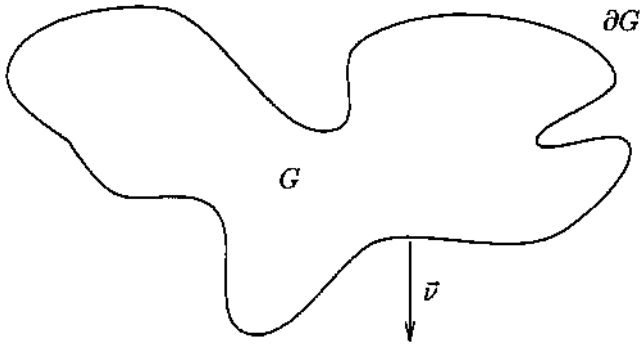

Figure 9. Arbitrary region G with boundary ∂G

As usual, we distinguish between three types of boundary conditions:

(1) **Dirichlet conditions** are fixing the temperature field on the boundary surface.

$$T(\vec{x})\Big|_{\partial G} = g(\vec{x}) \quad \forall x \in \partial G \tag{16}$$

(2) **Neumann conditions** are fixing the flux through the surface.

$$\vec{\nu}\,\vec{j}_T(\vec{x})\Big|_{\partial G} = -\lambda(T)\,\frac{\partial}{\partial \nu}T\Big|_{\partial G} = g(\vec{x}) \quad \forall x \in \partial G \tag{17}$$

(3) **Poincaré conditions** are fixing the flux through the surface by means of the temperature itself.

$$\vec{\nu}\,\vec{j}_T(\vec{x})\Big|_{\partial G} = -\lambda(T)\,\frac{\partial}{\partial \nu}T\Big|_{\partial G} = g(\vec{x})\,T(\vec{x})\Big|_{\partial G} \quad \forall x \in \partial G \tag{18}$$

Thereby g is an arbitrary function.

While proceeding we call the finite set of grid vertices G_d. The set of boundary vertices is called ∂G_d Now we are interested in the discrete version of the boundary conditions.

3.2.1 Dirichlet conditions

Owing to the application of the vertex stored method, there are temperature values stored on the boundaries. Thus the discretisation of (16) is a very obvious task

$$T(\vec{x}) = g(\vec{x}) \quad \forall x \in \partial G_d. \tag{19}$$

The temperature stored in the boundary vertices is determined by the boundary condition itself. There is no need to recalculate them. They enter the equations just as constants. In terms of equation (12): The boundary temperatures are entering the repetitive scheme only on the right hand side; there is no derivative of them in the Newton matrix.

3.2.2 Neumann conditions

To handle Neumann conditions, the temperature in the vertex has to be calculated. While integrating the heat conduction equation over the control volume a new kind of term appears due to the treatment of boundaries. With the help of Figure 10, we see immediately that we have to respect the additional flux through the boundaries. In the numerical case this flux is written as

$$\int_{\partial V_i \cap \partial G} \vec{j}_T \, \mathrm{d}\vec{\sigma} \cong \left(|\vec{n}_L| + |\vec{n}_R|\right) g(\vec{x}_I)$$

with

$$\vec{n}_L = -\frac{3I_r + L_r}{8} \vec{IL}_\perp; \quad \vec{n}_R = +\frac{3I_r + R_r}{8} \vec{IR}_\perp.$$

A special case

$$g \equiv 0$$

is also called an adiabatic case, since no flux is passing through the boundary surface. The implementation of this condition is cogitably easy: no additional terms appear. That means, those vertices which are on the boundary and are taken to be calculated, fulfil automatically adiabatic boundary conditions.

3.2.3 Poincaré conditions

After the upper inspection, it is no problem to write down the discrete type of Poincaré conditions which are very useful to describe the flow through small walls.

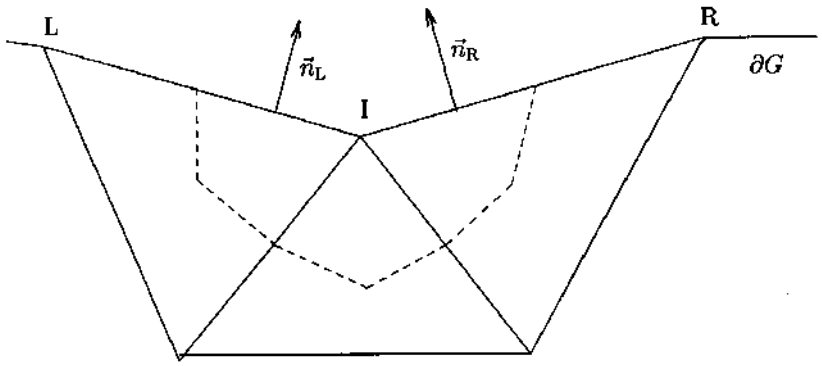

Figure 10. Additional surface integral on ∂G

$$\int_{\partial V_I \cap \partial G} \vec{j}_T \, d\sigma \cong \left(|\vec{n}_L| + |\vec{n}_R|\right) g(\vec{x}_I) \, T_I$$

The main difference is that Poincaré conditions yield to additional terms in the iteration matrix, since the additional fluxes are temperature dependent. The expansion to nonlinear Poincaré conditions (e.g. heat loss by radiation) is obvious.

4. Conclusion

An ideal discretisation scheme for partial differential equations should possess certain desirable properties. It should:

- work in arbitrary geometries;
- preserve symmetry and monotonicity properties of discretised operators;
- be conservative;
- work also on rough grids (multi-grid solvers, care of calculation capacity);
- allow convenient enforcement of boundary and interface conditions;
- permit adaptive mesh construction;
- be free of dimensional restrictions.

Of course, any concrete discretisation does not satisfy all of the above requirements. In this paper a not too circumstantial way was presented to fulfil monotonicity properties of the physical problem even in the discretised numerical case on rough grids. Owing to the use of unstructured grids most of the upper requirements are fulfilled as well. The expansion to higher dimensional space is trivial.

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