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Properties of numeric schemes for stiff transport models

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1. Introduction

It is known that the anomalous transport in fusion devices is governed by gradient-driven instabilities and is characterised by an offset linear dependence of the heat and particle fluxes on the corresponding gradients. The dependence is very strong so that a small increase in gradients causes a huge enhancement of fluxes thus giving rise to the so called stiff transport. This feature makes the standard numeric schemes that imply Fick's law of diffusion strongly unstable and leads to extremely small time steps in transport simulations. A modification of the standard finite difference scheme was recently suggested [1] that eliminates this kind of numerical instability. It has been shown that the time step for stiff transport models can be increased by several orders of magnitude. Generalisation to more advanced numeric schemes and to a system of parabolic equations is straightforward.

On the other hand, this scheme modification introduces an additional numerical error that disappears at the steady state but can noticeably affect the run flow in transient processes. Although the two requirements, the numerical stability and the numerical accuracy, are compulsory for any numerical scheme they can be considered independently because they are well separated in physical meaning and in numerical restrictions. Stability, as the most limiting of the two factors, was in details considered in our previous paper [1]. In this presentation we concentrate on the numerical accuracy, the issue that has not been properly addressed in [1].

2. Problem of stability and the numerical scheme

For a stiff transport there are two different limits on the simulation time step τ imposed by the stability and accuracy requirements. The two limits are essentially independent and a gap between those is so large that lifting the stability restriction allows to increase the time step by three or more orders of magnitude before the accuracy problem comes to the fore. Nevertheless, at some point the accuracy restriction comes into play and it becomes necessary to evaluate all possible negative consequences of the spoiled numerical accuracy. In [1], all practical calculations have been done for the realistic tokamak configuration with the GLF23 transport model [2] and it was demonstrated that the numerical stability can be drastically improved when an additional small term is added to the standard numerical approach. The general consideration was possible because the numerical instability cannot remain invisible. Once it appears it prevents any kind of reasonable modelling and at the developed phase destroys the run. In opposite, insufficient numerical accuracy is not that obvious therefore we will study the numerical errors making use of a simplified model problem.

Consider the simplified quasi-cylindrical diffusion equation for the function $u = u(x,t)$

$$\frac{\partial u}{\partial t} = \frac{1}{x}\frac{\partial}{\partial x}\left(xD\frac{\partial u}{\partial x}\right) + S, \quad D = D_0 + D_{an} = D_0 + \begin{cases} D_1 u\,(\eta - \eta_{cr}), & \text{if } \eta \geq \eta_{cr}, \\ 0, & \text{if } \eta < \eta_{cr}. \end{cases} \qquad (1)$$

Here, u is a generic plasma parameter as density, temperature, etc., $D = D(x,u,u_x)$ is the diffusion coefficient and $S = S(t,x,u)$ is a source term. The flux $q = -Du_x = q_0 + q_{an}$ includes the [neo]classical and anomalous parts. We introduced a logarithmic gradient $\eta = -u_x/u$ of the quantity u so that $q = uD\eta$. The anomalous flux q_{an} is related to a gradient driven instability where η_{cr} an instability threshold. This model equation Eq.(1) possesses all characteristic properties of the stiff transport and will be used below to elucidate main numerical properties and difficulties.

As a numerical scheme we employ a simple backward differencing in time and second order central difference in space with the accuracy $\mathcal{O}(\tau) + \mathcal{O}(h^2)$, τ and h being the time and space grid sizes respectively. For a non-stiff transport the scheme gives reasonable results for the time step of order $10^{-2}a^2/D \approx 10^{-2}$ s. If the scheme is applied for a typical stiff problem then the time steps drops to 10^{-5} s or lower making this way of simulation impracticable.

In [1], it was proposed to add an auxiliary flux in Eq.(1) so that

$$q = q_{cl} + q_{an} + q_{aux}, \qquad q_{aux} = V_{aux}\underline{u} - D_{aux}\underline{u_x}, \qquad V_{aux} = D_{aux}\frac{u_x}{u}. \qquad (2)$$

Difference representation of the flux q_{aux} is done in such a way that the two underlined terms in are approximated implicitly and all other terms explicitly. The scheme modification means that the same term is added as a diffusion and subtracted as an advection. Differentially, the net flux q_{aux} is identically equal to zero for arbitrary D_{aux}. Its numerical implementation is nonzero and produces strong stabilising effect that is explained in Fig. 1(b). The new scheme implies the flux dependence that is shown by the dashed line. If D_{aux} is large enough then the slope of the dashed line is higher than that of the physics dependence $q(\eta)$ (solid line in Fig. 1(b)) and the numerical process becomes stable.

There is an alternative way to get a similar stabilising effect. One can add the diffusion term $(D_{aux}u_x)_x$ to Eq. (1) implicitly and subtract it as a source (explicitly). In order to distinguish the both approaches we shall call them DA (diffusion–advection) and DS (diffusion–source) schemes. As mentioned above the modified schemes allow to increase the time step by a factor of up to 10^4 without any evidence of the instability. The time step enhancement grows rapidly with increasing D_{aux}. However, it is clear that a penalty for the improved stability is a loss of accuracy.

3. Numerical accuracy

Making the Taylor expansion of the different numerical approximations of Eqs. (1),(2) one can find numerical error introduced by the both schemes. The errors can be represented as fluxes

$$q^{err}_{DA} = -\tau D_{aux}u\,(\ln u)_{xt} + \mathcal{O}(h^2) + \mathcal{O}(\tau^2), \qquad q^{err}_{DS} = -\tau D_{aux}u_{xt} + \mathcal{O}(h^2) + \mathcal{O}(\tau^2), \quad (3)$$

or as sources $xS^{err} = (xq^{err})_x$. The expressions (3) show that modification (2) is equivalent to adding a higher order space-time derivative with a small factor τ in front of it. Having in mind that the numerical instability manifests itself as short-wave oscillations with the opposite signs in the adjacent grid cells one can understand that the additional terms suppress these parasitic modes and thus produce a stabilising effect.

By approaching a steady state, the errors (3) vanish although the numeric scheme remains stable. This property is very useful for parametric studies and for scenario assessment when only a steady state solution is of interest. On the other hand, all transient processes can be appreciably affected by the error. Therefore, control of the instant error is necessary for evaluating the quality of the computation. For a simple and straightforward evaluation of the error one can compare S^{err} with the actual source term S in Eq. (1). This gives a rough estimate of the disturbance introduced due to the numerical error.

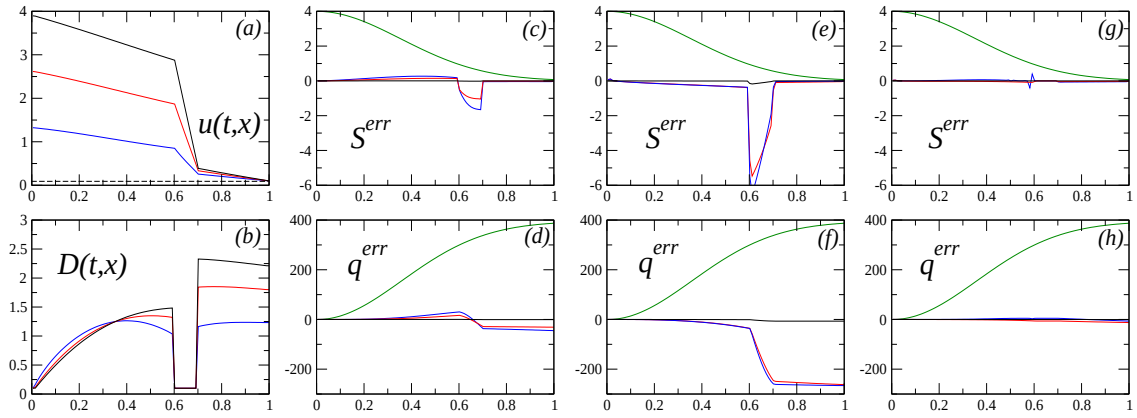

Fig. 1. Time evolution of the functions $u(t,x)$ (a), diffusion coefficient $D(t,x)$ (b). The local error in the source form S^{err} is shown in (c), (e) and (g). The same quantity in the form of flux (i.e. integrated over x is shown in (d), (f), and (h), respectively. Radial profiles are shown for the times $t = \tau_c/3$ (blue), $t = \tau_c$ (red), $t = 5\tau_c$ (black). Green curves show the function S and its integral q.

Fig. 1 illustrates the discussed behaviour. It shows profiles of $u(t,x)$, $D(t,x)$ and numerically introduced errors calculated with Eq. (1). Here $D_0 = 0.1$, $D_1 = 1$, $\eta_{cr} = 1$, $S(x) = 4\exp(-x^2)$. In order to simulate the internal transport barrier (ITB) the anomalous transport D_{an} was set to zero in the range $0.6 < x < 0.7$. In all calculations the spatial grid of 100 cells was used and the time step τ was fixed at $\tau = 10^{-2}$. The quantity D_{aux} was taken in the form $D_{aux} = Cu(t,x)$. The greater is the multiplier C, the stronger is the stabilising effect and the larger time step is possible. Moreover, above a certain value of C the computations become unconditionally stable [1]. On the other hand, Eq. (3) shows that the error grows with both C and τ. Therefore, minimisation of the error requires to minimise the product τD_{aux}. In our example, the constant multiplier $C = 0.5$ has been selected as the minimum value that provides a stable solution of Eq. (1) with the given time step $\tau = 10^{-2}$. For comparison: at $D_{aux} = 0$, the stability condition limits the time step to a much smaller value $\tau = 5 \times 10^{-5}$.

The time evolution is shown starting at the time $t = \tau_c/3$ where τ_c is the confinement time calculated at steady state. At this time the numerical errors reach maximum value and then

drop to zero at steady state (Fig. 1(c-h)). Figures 1 (a), (b), (c) and (d) show the DA algorithm, (e) and (f) the DS algorithm. As mentioned, in both cases the same value of $D_{aux} = 0.5u$ was applied. For the model (1), the DA algorithm (c-d) produces noticeably smaller errors then the DS algorithm (e-f). However, it does not mean that the latter is of no use. Indeed, it is seen that in the range $x < 0.6$ the quantity S^{err} has different signs for different algorithms. This suggests an idea to use a linear combination of the both in order to minimise the error.

The next remark is that the error is especially large in the ITB domain. This observation is of no surprise because no correction is needed in the range where $D_{an} = 0$. The combined algorithm has been constructed where DA and DS corrections are used in the proportion 3:2 and both are suppressed in the interval $0.6 < x < 0.7$. The results are shown in Fig. 1 (g-h). It is seen that for this particular case the numerical error can be reduced to a negligible level. However, in Fig. 1 (g) one can see an oscillatory behaviour of S^{err} at $x = 0.6$. This is typical for a boundary layer where a strong variation of D (or D_{aux}) takes place.

It should be noted that a realistic case, where the stiffness depends on the gradient, $D_1 = D_1(\eta)$, may be much more complicated. Sometimes one can see intermittent bursts of this instability or it exists continuously but stays local. An unstable feedback can develop when the boundary point jumps to the next grid node and back. When the instability threshold is exceeded by a larger margin the local short-wave perturbation can expand and affect a wider zone. All types of this unstable behaviour affect the accuracy of the solution and can distort formation or evolution of ITBs. In this situation usage of stepwise D_{aux} as in Fig. 1 (g-h) does not help. In practical modelling, most reliable results have been always obtained with a constant or weakly varying D_{aux}. Increasing D_{aux} suppresses the oscillations but increases the error.

As discussed the choice of D_{aux} and τ depends on the two contrary conditions: stability and accuracy. However, there is a practically significant case when the second condition does not play a decisive role. If the final goal of computation is the steady state then the numerical error during the transient phase can be ignored and it is only needed to check if the error (3) drops to the acceptable level at the end of the run.

Working at the stability threshold is potentially dangerous because this type of numerical instability has some unusual features. Specific aspect of it is that once the instability arises it can be seen first on the gradient u_x. Only at a high enough amplitude it affects also the function u. If an automated time step control is based on the behaviour of u it can interactively sustain the instability near (above) the threshold when u seems to be unaffected but u_x exhibits a low level noise. As a matter of fact, this visibly smooth and unspoiled u can be wrong because D_{an} amplifies all uncertainties in u_x. Even if a noise in u_x has zero mean deviation it can be not the case for the average D_{an}. An influence on u is then unpredictable. This and some other open issues related to the stiff transport require a thorough study of the numerical schemes in relation with particular transport models.

References

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