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Achievable efficiency of numerical methods for simulations of solar surface convection

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ABSTRACT

We investigate the achievable efficiency of both the time and the space discretisation methods used in Antares for mixed parabolic–hyperbolic problems. We show that the fifth order variant of WENO combined with a second order Runge–Kutta scheme is not only more accurate than standard first and second order schemes, but also more efficient taking the computation time into account. Then, we calculate the error decay rates of WENO with several explicit Runge–Kutta schemes for advective and diffusive problems with smooth and non-smooth initial conditions. With this data, we estimate the computational costs of three-dimensional simulations of stellar surface convection and show that SSP RK(3,2) is the most efficient scheme considered in this comparison.

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The simulation code Antares [1] was developed for the simulation of solar and stellar surface convection. Recently it has also been applied to many other astrophysical problems (e.g. [2,3]).

In this code, the Navier–Stokes equations usually without magnetic field and with radiative transfer (radiation hydrodynamics, RHD) are solved in the form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1a}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \rho \mathbf{g} + \nabla \cdot \tau, \tag{1b}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u} (E + p)) = \rho (\mathbf{g} \cdot \mathbf{u}) + \nabla \cdot (\mathbf{u} \cdot \tau) + Q_{\text{rad}}. \tag{1c}$$

The meaning and units of all variables are shown in Table 1. An equation of state must be specified to complete this set of equations. The viscous stress tensor $\tau = \left(\tau_{i,j}\right)_{i=1,2,3}$ is given by

$$\tau_{i,j} = \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{i,j} (\nabla \cdot \mathbf{u}) \right) + \zeta \, \delta_{i,j} (\nabla \cdot \mathbf{u}) . \tag{2}$$

$\mathbf{g}$ is the gravity vector and Q_{rad} is the radiative heating rate describing the energy exchange between gas and radiation. $\delta_{i,j}$ is the Kronecker symbol. η and ζ are the first and second coefficients of viscosity.

We can rewrite Eq. (1) as

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F}_{\text{adv}} = \nabla \cdot \mathbf{F}_{\text{visc}} + \mathbf{S} \tag{3a}$$

with

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ E \end{pmatrix}, \qquad \mathbf{F}_{\text{adv}} = \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + p \, \text{Id} \\ \mathbf{u} (E + p) \end{pmatrix},$$
$$\mathbf{F}_{\text{visc}} = \begin{pmatrix} 0 \\ \tau \\ \mathbf{u} \cdot \tau \end{pmatrix}, \qquad \mathbf{S} = \begin{pmatrix} 0 \\ \rho \mathbf{g} \\ \rho (\mathbf{g} \cdot \mathbf{u}) + Q_{\text{rad}} \end{pmatrix}. \tag{3b}$$

$\mathbf{Q}$ is the vector containing the conserved quantities and Id is the identity matrix. We call the terms collected in $\mathbf{F}_{\text{adv}}$ the *advective* or *inertial* part and in $\mathbf{F}_{\text{visc}}$ the *viscous* part of the Navier–Stokes equations. All first derivatives are contained in $\nabla \cdot \mathbf{F}_{\text{adv}}$, all second order terms in $\nabla \cdot \mathbf{F}_{\text{visc}}$. We note that $\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F}_{\text{adv}} = 0$ is of hyperbolic type, whereas $\frac{\partial \mathbf{Q}}{\partial t} - \nabla \cdot \mathbf{F}_{\text{visc}} = 0$ is a parabolic system.

1. Discretisation and numerical methods

Following the *method of lines* approach of discretising space and time separately [4,5], Eq. (7) are discretised in space only and converted to

$$\frac{\partial \mathbf{Q}}{\partial t} = \text{L} (\mathbf{Q}) , \tag{4}$$

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Table 1
Variable names, meaning and CGS units as used in this paper. Note that x denotes the vertical direction. Vectors are written in bold face. The velocity vector is $\mathbf{u} = (u, v, w)^T$.

Variable	Meaning	Unit (CGS)
ρ	gas density	$\mathrm{g\,cm^{-3}}$
T	temperature	K
p	pressure	$\mathrm{dyn\,cm^{-2}}$
u	x velocity (vertical)	$\mathrm{cm\,s^{-1}}$
v	y velocity (horizontal)	$\mathrm{cm\,s^{-1}}$
w	z velocity (horizontal)	$\mathrm{cm\,s^{-1}}$
Q_{rad}	radiative heating rate	$\mathrm{erg\,s^{-1}\,cm^{-3}}$
v_{snd}	sound speed	$\mathrm{cm\,s^{-1}}$
E	total energy	$\mathrm{erg\,cm^{-3}}$
e	internal energy	$\mathrm{erg\,cm^{-3}}$
ϵ	specific internal energy	$\mathrm{erg\,g^{-1}}$
η	dynamic viscosity	$\mathrm{g\,cm^{-1}\,s^{-1}}$
ζ	second (bulk) viscosity	$\mathrm{g\,cm^{-1}\,s^{-1}}$

where L is the operator resulting from the spatial discretisation of $-\nabla \cdot \mathbf{F}_{\mathrm{adv}} + \nabla \cdot \mathbf{F}_{\mathrm{visc}} + \mathbf{S}$. In principle, the integration of this equation can be performed with any numerical method for solving ordinary differential equations, in particular Runge–Kutta methods, provided they are numerically stable, although further properties (such as positivity, e.g., of T or E) may be required (cf., for instance, Kupka et al. [6]).

The spatial discretisation is done separately for $\mathbf{F}_{\mathrm{adv}}$ and $\mathbf{F}_{\mathrm{visc}}$ as defined in Eqs. (3). In optically thin regions the radiative heating rate Q_{rad} is a source term and is calculated separately by the radiative transfer solver as described in Muthsam et al. [1]. In optically thick regions, the diffusion approximation

$$Q_{\mathrm{rad}} = \nabla \cdot (\kappa \nabla T) \tag{5}$$

is valid such that we can include Q_{rad} in the $\mathbf{F}_{\mathrm{visc}}$ term.

For $\mathbf{F}_{\mathrm{adv}}$, the WENO finite difference scheme is employed [7–9]. The WENO scheme is a highly efficient shock-capturing scheme which we consider here in its fifth order variant called WENO5. In the context of solar surface convection simulations, its superiority in terms of accuracy compared to other high-order schemes was shown in Muthsam et al. [10]. Its main part, the fifth order accurate reconstruction operator, is summarised in Algorithm 3.

For $\mathbf{F}_{\mathrm{visc}}$, the fourth-order accurate scheme from Happenhofer et al. [11] is used. First, we outline the procedure for the one-dimensional diffusion equation

$$\frac{\partial \phi}{\partial t} - D\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial \phi}{\partial x}\right) = 0 \tag{6}$$

with the constant coefficient of diffusion D. In one spatial dimension and on an equidistant Cartesian grid, the outer derivative is approximated by

$$\frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial x}\right)(x_i) = \frac{\frac{\partial \phi}{\partial x}\left(x_{i+\frac{1}{2}}\right) - \frac{\partial \phi}{\partial x}\left(x_{i-\frac{1}{2}}\right)}{\delta x} \tag{7a}$$

with constant grid spacing δx. Then, the inner derivative is calculated by

$$\frac{\partial \phi}{\partial x}\left(x_{i-\frac{1}{2}}\right) = \frac{\phi_{i-2} - 15\phi_{i-1} + 15\phi_i - \phi_{i+1}}{12\,\delta x}, \tag{7b}$$

leading to a fourth-order accurate approximation. Here, $\phi_i = \phi(x_i)$.

Similar procedures can be applied to any second-order term, in particular to $\mathbf{F}_{\mathrm{visc}}$. Special care has to be taken for mixed derivatives. In the two-dimensional case and considering only the $\mathbf{F}_{\mathrm{visc}}$ terms, we arrive at

$$\frac{\partial}{\partial t}(\rho u) = \frac{\partial}{\partial x}\left(\left(\zeta + \frac{4}{3}\eta\right)\frac{\partial u}{\partial x} + \left(\zeta - \frac{2}{3}\eta\right)\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(\eta\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right) \tag{8}$$

by virtue of Eqs. (1) and (2). The outer derivatives are replaced by a finite difference, evaluating the inner function at the half-integer nodes. Therefore, we need the terms inside the spatial derivatives in (8) at $(i-\frac{1}{2}, j)$ and at $(i, j-\frac{1}{2})$. $\frac{\partial u}{\partial x}$ at $(i-\frac{1}{2}, j)$ and $\frac{\partial v}{\partial y}$ at $(i, j-\frac{1}{2})$ can be calculated directly by formula (7b). Then, the coefficient functions must be interpolated to the half-integer grid. To fourth-order accuracy,

$$\eta_{i-\frac{1}{2},j} = \frac{-\eta_{i-2,j} + 7\eta_{i-1,j} + 7\eta_{i,j} - \eta_{i+1,j}}{12}, \tag{9}$$

assuming that the variable is given as a cell average. To calculate $\frac{\partial v}{\partial y}$ at the half integer index $\left(i-\frac{1}{2}, j\right)$, we calculate the derivative at the cell centre by

$$\frac{\partial v}{\partial y}|_{i,j} = \frac{v_{i,j-2} - 8v_{i,j-1} + 8v_{i,j+1} - v_{i,j+2}}{12\,\delta y}, \tag{10}$$

and then interpolate the result to $\left(i-\frac{1}{2}, j\right)$ according to formula Eq. (9). The computation of $\frac{\partial u}{\partial x}$ at $\left(i, j-\frac{1}{2}\right)$ is done analogously. The resulting procedure is fourth-order accurate.

After the spatial discretisation step, the Eq. (1) are transformed to the form Eq. (4). Since Eq. (4) is an ordinary differential equation, we can use Runge–Kutta schemes to integrate it.

We follow Gottlieb et al. [12] in defining some basic properties of Runge–Kutta schemes.

Definition 1. Let an initial value problem of the form

$$\phi'(t) = \mathrm{L}(\phi(t)), \qquad \phi(0) = \phi_0, \tag{11}$$

be given. An *explicit s-stage Runge–Kutta* scheme is an integration scheme of the form

$$\begin{aligned} &\phi^{(0)} = \phi^n, \\ &\phi^{(i)} = \sum_{k=0}^{i-1}\left(\alpha_{i,k}\,\phi^{(k)} + \delta t\,\beta_{i,k}\,\mathrm{L}(\phi^{(k)})\right), \\ &\quad \alpha_{i,k} \geq 0,\ i = 1, \ldots, s, \\ &\phi^{n+1} = \phi^{(s)}, \end{aligned} \tag{12}$$

where $\phi^n = \phi(t_n)$ and the time step δt is given by the CFL condition.

Definition 2. Assume that L results from the discretisation of a spatial operator and let a seminorm $\|\cdot\|$ be given. Following Wang and Spiteri [13], a Runge–Kutta method of the form (12) is called strong stability preserving (SSP) if for all stages i, $i = 1, 2, \ldots, s$,

$$\|\phi^{(i)}\| \leq \|\phi^n\| \tag{13}$$

with a CFL restriction on the time step δt.

The *total variation diminishing (TVD)* property [7] is a special case of this definition. It results from inserting the *total variation* norm of ϕ at time t_n,

$$\mathrm{TV}(\phi^n) = \sum_j |\phi^n_{j+1} - \phi^n_j|, \tag{14}$$

in (13).

In this paper, we consider four explicit time integration schemes: the first-order Euler forward method, the second-order two-stage TVD2 and the third-order three-stage TVD3 scheme from Shu and Osher [7]. The fourth explicit scheme is the second-order three-stage scheme from Kraaijevanger [14], further studied in Ketcheson et al. [15] and Kupka et al. [6], called SSP RK(3,2).

The TVD2 and TVD3 (total variation diminishing) schemes were also analysed with respect to their SSP (strong stability preserving) properties by Kraaijevanger [14]. Their coefficients were first

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