Advances in direct deconvolution modeling of subgrid-scales for flows with discontinuities

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1. Motivation and objectives

We develop a method for a unified treatment of flow discontinuities and turbulent subgrid flow scales using the filtering approach. For the filtered evolution equations, the solution is smooth and can be solved for by standard central-difference schemes without special considerations of discontinuities. The approach is based on an approximate regularized deconvolution of the filtered solution to obtain a sufficiently accurate representation of the smoothed nonlinear combination of discontinuous fields, e.g., the convection term. For stable integration the evolution equations are supplemented by a relaxation regularization based on a secondary filter operation. We detail the approach and demonstrate its efficiency with the inviscid Burger's equation, the isothermal shock problem, and the one-dimensional Euler equations.

In large-eddy simulations (LES) non-resolved scales (here we restrict ourselves to spatial scales) are removed by convolving the underlying nonlinear transport equation with a filter. As a consequence, correlations of non-filtered quantities arise from the nonlinear terms and require closure. A closure would be trivial if the filtering operation could be exactly inverted. An inverse-filter operation, however, is necessarily ill-conditioned, which reflects the fact that information about non-resolved scales is required.

Predictions of turbulent subgrid-scale stresses by models of eddy-diffusivity type do not correlate well with the real subgrid-scale stresses. This led recently to an increased interest in deconvolution-type models. The first of such models was based on Taylor expansions in the expressions for the filtered product of the velocity components (Leonard, 1974) and on the assumption of scale-similarity (Bardina *et al.*, 1983). More recently, a deconvolution approach from a polynomial approximation of the filter kernel was constructed (Shah & Ferziger, 1995, Geurts, 1997, Kuerten *et al.*, 1999). Another approach which clearly exhibits the deconvolution structure was proposed by Domaradzki & Saiki (1997) where the resolved scales are deconvolved directly. The non-resolved scales are approximated from the instantaneous nonlinear interaction of the resolved scales. Without recourse to physical modeling, Stolz & Adams (1999) introduced an approximate deconvolution technique (ADM) based on truncated series expansion of the inverse-filter kernel. *A priori* tests for direct numerical simulation (DNS) data of supersonic compression ramp flow give correlations in excess of 95% for subgrid-scale stresses (Stolz *et al.*, 1999a). Excellent agreement with DNS was demonstrated in *posteriori* tests for compressible homogeneous turbulence (Stolz & Adams, 1999) and for incompressible channel flow (Stolz *et al.*, 1999b).

Direct or approximate deconvolution techniques lend themselves also to the reconstruction of non-turbulent subgrid scales and thus provide a way for a unified

treatment of turbulent and non-turbulent subgrid-scales. Among the latter are shocks, contact discontinuities, and sharp fluid interfaces, which we call *genuine subgrid-scales* since they remain subgrid-scales independently of numerical resolution. We address fundamental issues of approximate regularized deconvolution following an approach suggested in Adams *et al.* (1998) when applied to nonlinear transport equations which allow for discontinuous solutions. Generic test cases are the Burger's equation and the one-dimensional Euler equations.

For a given numerical discretization on a partitioning of the real line with constant spacing h, we discern between *resolved scales* with wavenumbers $|\xi| \leq \xi_C$, *represented scales* $\xi_C < |\xi| \leq \xi_N = \pi/h$, and *non-represented scales* $|\xi| > \xi_N$. ξ_N is the Nyquist wavenumber, the smallest scale which can be represented on the grid. For nonlinear conservation laws the interaction of represented scales with non-represented scales is essential to provide sufficient entropy dissipation in order to ensure that the solution of the filtered conservation law (which can be interpreted as a specific discretization of the continuous non-filtered conservation law) converges to the correct entropy solution for $h \to 0$, the filter-width Δ being proportional to h (Lax, 1973). This can be achieved by regularizing the filtered evolution equation with an additional term providing entropy dissipation, often formulated as artificial viscosity or super-viscosity, such as the von Neumann-Richtmyer artificial viscosity, for instance (e.g., Hirsch, 1990). An illustrative example is the periodic N-wave solution to the inviscid Burger's equation, where insufficient entropy dissipation gives rise to an incorrect positive-jump discontinuity in the wake of the main negative-jump discontinuity. An other example is isotropic turbulence, governed by the three-dimensional Navier-Stokes equations, in the limit of vanishing viscosity, where the appearance of the so-called equi-partition spectrum is usually observed for non-dissipative numerical discretizations without providing sufficient subgrid-scale dissipation (e.g., Lesieur, 1997). The correct vanishing-viscosity solution can be recovered in this case by adding a regularization such as a proper eddy-viscosity term, e.g. the Smagorinsky model (e.g., Lesieur, 1997), which has a striking similarity to the von Neumann-Richtmyer artificial viscosity. The main effect of an eddy-viscosity regularization is to provide a sufficient amount of energy dissipation (Jimenez & Moser, 1999, Jimenez, 1999). More refined and more elaborate forms of subgrid-scale models have been proposed; for a recent summary refer to Moin (1997) and Lesieur & Metais (1996).

These observations suggest a relation between subgrid-scale models which approach the closure problem from a physical point of view by incorporating into the model as many properties known from the underlying mathematical model as possible, and numerical techniques which regularize the discretization of a conservation law in order to ensure convergence to the correct entropy solution. We note that it has been successfully attempted for some flow configurations to replace a subgrid-scale model entirely by artificial viscosity introduced by the underlying numerical method, which is then directly linked to the truncation error (Boris *et al.*, 1992). Detailed investigations of this approach by Garnier *et al.* (1999) show, however, that it lacks general applicability.

In our approach we try to bridge physical and numerical subgrid-scale modeling by introducing a model which extracts from the represented scales as much information on the resolved scales as possible and which also ensures sufficient energy dissipation. The former is achieved by a deconvolution operation on the represented scales, the latter by a relaxation term employing a secondary filter operation on the represented non-resolved scales. We point out that the regularization when viewed in Fourier dual space has a resemblance with spectral super-viscosity regularizations (Tadmor, 1993). In real space, however, it is a lower order perturbation of the underlying equations and leaves the type of the equations unchanged. This is a considerable advantage over higher order regularizations since the well-posedness conditions for the underlying conservation law transfer to the regularized system (Gustafsson, 1995).

2. Accomplishments

2.1 Filtering approach

For a given generic nonlinear transport equation

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0 \ , \quad 0 \leq x \leq L \tag{1}$$

a filtered transport equation

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial F(\overline{u})}{\partial x} = \mathcal{G} \tag{2}$$

is obtained by convolution with a homogeneous filter

$$\overline{u}(x) = \int_{-\infty}^{+\infty} G(x - x')u(x')dx' = G * u \ , \tag{3}$$

where

$$\mathcal{G} = \frac{\partial F(\overline{u})}{\partial x} - G * \frac{\partial F(u)}{\partial x}$$

is an error term due to the filtering. Eq. (2) is the modified differential equation for $\bar{u}$, the solution of which would be identical to the filtered solution of (1) if $\mathcal{G}$ could be computed exactly.

Numerical discretizations of (2) carry wavenumbers ξ up to the Nyquist wavenumber $\xi_N = \pi/h$, where $h = L/N$ is the uniform grid-spacing and N is the number of intervals into which the domain $[0, L]$ is partitioned. We call ξ_N the *numerical cutoff wavenumber*. If we apply the filter operation to the solution $\bar{u} = G * u$, we discern between wave numbers $0 \leq |\xi| \leq \xi_C$, which we consider to be *resolved*, and wavenumbers $\xi_C < |\xi| \leq \xi_N$, which we consider to be *non resolved*, and we call ξ_C the *subgrid cutoff wavenumber*. For low-pass filters other than the spectral cutoff filter, the determination of ξ_C is a matter of definition, see Eq. (8). It is obvious that the ratio ξ_C/ξ_N should be chosen such that ξ_C can be considered to be well

resolved by the underlying numerical discretization scheme. For finite-difference schemes the relevant error measure is given by the modified wavenumber concept (Vichnevetsky & Bowles 1982).

If we assume that u can be recovered exactly from $\bar{u}$ at every time instant, then the discretization of (2) reduces to a discretization of (1) with a post-processing filter G applied during the time integration. It is known that the solution of the discretized Eq. (2) in this case fails to converge to the correct entropy solution (Tadmor, 1989). Accordingly, an additional regularization of Eq. (2) is required. Tadmor (1990, 1993) proposed several spectral viscosity and spectral super-viscosity regularizations. The disadvantage of these regularizations is that they either amount to adding higher-order terms or to convolution operations in real space. For a non-periodic finite domain the former can require different boundary conditions for the modified form of (1) if the artificial viscosity does not vanish at the boundaries (Boyd, 1998).

In this paper we propose a low order regularization in the form of a relaxation term

$$\mathcal{R} = -\chi(\bar{u} - G_2 * \bar{u}) \tag{4}$$

where χ is the inverse of the relaxation time and $G_2(x)$ is a secondary filter of convolution type (3). The equation which is solved numerically for $\bar{u}$ is then

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial F(\overline{u})}{\partial x} = \mathcal{G} + \mathcal{R} \ , \tag{5}$$

with a suitable approximation for $\mathcal{G}$.

It is illustrative to recall that filtering, de-filtering, and discretization implicitly contain restrictions and extensions of the representing function spaces. This can be seen easily using a Fourier dual space representation assuming that a Fourier transform exists. The same holds, however, also for more general cases. The solution of (1) is in $\mathcal{H}_\infty$, which we call the space of all square-integrable functions. A discretization of (1) which represents u by u_N on a grid with spacing h restricts the solution to $\mathcal{H}_{\xi_N}$, the space of all functions, the Fourier-transforms of which have a support $|\xi| \leq \xi_N = \pi/h$ (band-limited functions). Application of the filter $G(x)$ further restricts $\bar{u}_N$ to $\mathcal{H}_{\xi_G}$, where $[-\xi_G, \xi_G]$ is the support of the filter transfer function, and $\xi_G \leq \xi_N$. For the filter kernels used in this paper, it is always $\xi_G = \xi_N$. Note that, according to our definition of ξ_C, it is $\xi_C < \xi_N$, except for a sharp spectral cut-off. An approximate inverse solution of $G * u = \bar{u}_N$ will return some $\tilde{u}_N \in \mathcal{H}_{\xi_N}$ with $u = \tilde{u}_N + u'$, where $u' \in \mathcal{H}_\infty$. A quadratic nonlinear combination $\tilde{u}_N^2$, e.g., generates scales in $[-2\xi_N, 2\xi_N]$ which cannot be represented on the grid. Scales $\xi \notin [-\xi_N, \xi_N]$ contribute to aliasing errors. A subsequent application of the filter operation G restricts $G * (\tilde{u}_N^2)$ to $\mathcal{H}_{\xi_G}$. For the primary-filter operation we choose as kernel the Gauß function. In real space the filter is defined as

$$G(x) = 2\sqrt{\frac{2}{\pi}}\frac{1}{\Delta}e^{-8\frac{x^2}{\Delta^2}} \tag{6}$$

where Δ is the filter width. The Fourier transform of (6) is given by

$$\hat{G}(\xi) = e^{-\left(\frac{\Delta\xi}{4\sqrt{2}}\right)^2} \ . \tag{7}$$

We define the primary-filter width Δ as the length at which

$$\int_0^{\Delta} G(x)dx = \frac{1}{2} \ . \tag{8}$$

The cutoff wavenumber ξ_C is then given by

$$\xi_C = \frac{2\pi}{\Delta} \ .$$

$$\hat{G}_2(\xi) = e^{-\left(\frac{\Delta_2\xi}{4\sqrt{2}}\right)^{2p}} = G^p(\Delta_2) \ , \tag{9}$$

where Δ_2 is the filter width of the secondary filter. In general we will use $\Delta_2 = \Delta/2$ and $p = 6$.

The real-space filter kernel can be obtained from the inverse Fourier transform

$$G_2(x) = \mathcal{F}^{-1}(\hat{G}_2) \ . \tag{10}$$

Since we are not going to use the analytical expressions for the filter kernels but rather numerical approximations, we do not actually need to perform the inverse Fourier transform.

We require the discretized representations of the filters (6) and (10) to resemble closely the transfer function of the respective analytic filter kernels. The transfer functions of discretizations of (3) by standard quadrature formulas (trapezoidal rule or Simpson's rule, e.g.) usually exhibit a considerable error, in particular at wave numbers close to ξ_N. A convenient way for a more accurate numerical representation is to use a Padé filter (Lele, 1992, Pruett & Adams, 1999). We define a filter to be of order m if the first non-vanishing derivative of its transfer function (its Fourier transform) is of order m at $\xi = 0$. Let $\mathbf{f}$ be an $(N+1)$ vector containing the values of the grid function $f_i = f(x_i)$ obtained by sampling a continuous function $f(x)$ at a set of equally spaced nodes $x_j = x_0 + jh$, $0 \le j \le N$. Let $\overline{\mathbf{f}}$ denote the vector of filtered values obtained by applying the discrete filter $\mathbf{G}$ to $\mathbf{f}$, in matrix-vector notation $\overline{\mathbf{f}} = \mathbf{G}\mathbf{f}$. Here, we consider the special case in which $\mathbf{G} = \mathbf{M}_l^{-1}\mathbf{M}_r$, and $\mathbf{M}_l$, $\mathbf{M}_r$ are tridiagonal matrices. A one-parameter family of filters with $m = 2$ is given by

$$\alpha\overline{f}_{j-1} + \overline{f}_j + \alpha\overline{f}_{j+1} = af_j + \frac{b}{2}(f_{j-1} + f_{j+1}) \quad , \tag{11}$$

where $a = (1/2 + \alpha)$ and $b = a/2$. For a finite domain, various treatments are possible at the boundary points $j = 0$ and $j = N$. We will in general impose no filtering at domain-boundary points.

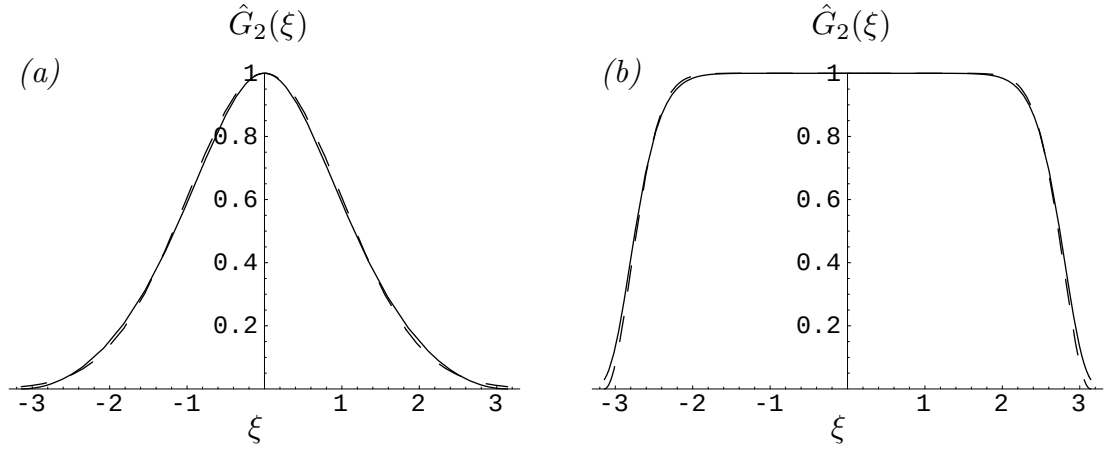

FIGURE 1. Transfer functions; (a) primary filter (6): ——— Padé discretization, - - - - exact $\Delta = 4h$; (b) secondary filter (10) : ——— Padé discretization, - - - - exact with $\Delta = 2h$ and $p = 6$.

The kernel of a Gauß filter (6) with filter width $\Delta = 4h$ is well approximated in Fourier space if one chooses $\alpha = -0.2$, Fig. 1a. For a secondary filter (10) with $\Delta_2 = 2h$ and $p = 6$, the exact transfer function $\hat{G}_2(\xi)$ is well approximated if one chooses $\alpha = 0.2$ in (11) and defines the discrete representation of G_2 by

$$\mathbf{G}_2 = \mathbf{M}_l^{-1}\mathbf{M}_r \sum_{\nu=0}^{6} (\mathbf{I} - \mathbf{M}_l^{-1}\mathbf{M}_r)^\nu \ ,$$

where $\mathbf{I}$ is the unit matrix. In the following we will call $G_N(x)$ and $G_{2N}(x)$ the discrete approximations of the corresponding continuous filters $G(x)$ and $G_2(x)$, respectively. Note that $\hat{G}_N(x)$ and $\hat{G}_{2N}(x)$ are bandlimited functions and thus have continuous real space representations $G_N(x)$ and $G_{2N}(x)$ using Whittaker's cardinal function (Vichnevetsky & Bowles 1982).

2.2 Subgrid-scale modeling

We introduce the operator $P_N u$, which projects $u \in \mathcal{H}_\infty$ onto $\mathcal{H}_{\xi_N}$. $\mathcal{G}$ can then be trivially re-written as

$$\mathcal{G} = \underbrace{\frac{\partial f(\bar{u})}{\partial x} - G * \frac{\partial f(P_N u)}{\partial x}}_{\mathcal{G}_1} + \underbrace{G * \left(\frac{\partial f(P_N u)}{\partial x} - \frac{\partial f(u)}{\partial x} \right)}_{\mathcal{G}_2} \ . \tag{12}$$

If we find an approximate inverse operator $\tilde{G}^{-1}$ for $G * u = \bar{u}$, given $\bar{u}$, which minimizes $\|P_N u - P_N \tilde{G}^{-1}\bar{u}\|$, the error in the computation of $\mathcal{G}_1$ is minimized. Since the range of $\tilde{G}^{-1}$ is $\mathcal{H}_N$, it is $P_N \tilde{G}^{-1}\bar{u} = \tilde{G}^{-1}\bar{u}$. The exact inverse of $G(x)$ does not exist in general since $1/\hat{G}(\xi)$ is unbounded by the Riemann-Lebesgue Lemma. It exists for such u for which $\hat{u}(\xi)/\hat{G}(\xi)$ is L_2-integrable.

Our approach is based on two procedures : (A) an accurate approximation of $\mathcal{G}$ in (5), (B) a relaxation regularization $\mathcal{R}$ in (5) to provide sufficient entropy dissipation to ensure convergence to the physically meaningful entropy solution. Procedure (A) is accomplished by an approximate deconvolution where we construct an approximate inverse of the discrete filter operator. Procedure (B) employs a secondary higher order filter, which leaves the resolved scales $|\xi| \leq \xi_C$ unaffected. All procedures are constructed such that they can be applied in a straightforward manner in real space. However, for convenience we will use the Fourier representation in the analysis.

The DDM approach is based on a direct deconvolution where a regularized inverse $\tilde{G}^{-1}(x)$ of the filter kernel $G(x)$ is used to obtain an approximation for u by $\tilde{u} = \tilde{G}^{-1}\bar{u}$. The transfer function $\hat{G}_N(\xi)$ of the discretization $\mathbf{G}$ of G for periodic domains is singular since it vanishes at $\xi = \pi/h$, Fig. 1a. On periodic domains the singularity can be removed by setting the Fourier mode $\hat{\bar{u}}(\pi/h)$ to zero (truncated singular-value decomposition). For $|\xi| < \pi/h$ one then obtains the approximately deconvolved variable $\tilde{u}$ from

$$\hat{\tilde{u}} = \frac{\hat{\bar{u}}}{\hat{G}_N(\xi)} \ , \quad |\xi| < \pi/h \ ; \quad \tilde{\bar{u}} = 0 \ , \quad |\xi| = \pi/h \ .$$

For nonperiodic domains an inverse of the discrete filter $\mathbf{G}$ exists if no filtering is imposed at the boundaries. In this case the spectrum of $\mathbf{G}$ is bounded away from zero on the negative real axis. Other regularization procedures such as truncated series expansion (Stolz & Adams, 1999), Tikhonov regularization, conjugate gradient method, etc., can be readily adapted from image processing (Bertero & Boccacci, 1998).

The term $\mathcal{G}_1$ in Eq. (12) can then be approximated by replacing the unfiltered quantities in $F(u)$ with $\tilde{u}$ and solving the following evolution equation for $\overline{u}$:

$$\frac{\partial \overline{u}}{\partial t} + G * \frac{\partial F(\tilde{u})}{\partial x} = 0 \ . \tag{13}$$

To cope with term $\mathcal{G}_2$ in Eq. (12), we propose a new type of regularization based on a relaxation term which employs a secondary higher-order filter operation. We want to point out that the potential of relaxation regularizations in general has been realized before (e.g., Jin & Xin 1995).

Here, we achieve regularization by adding a term

$$\mathcal{R} = -\chi(\bar{u} - G_2 * \bar{u}) \ , \tag{14}$$

where $\chi > 0$ is the inverse of the relaxation time and $G_2(x)$ is a secondary filter of deconvolution-type (3), to the right-hand side of (2). We use for $G_2(x)$ the secondary-filter kernel as defined by (10). The relaxation term has the following properties: the term is bounded in terms of u :

$$\|I - G_2\| \leq 1 \ ; \tag{15}$$

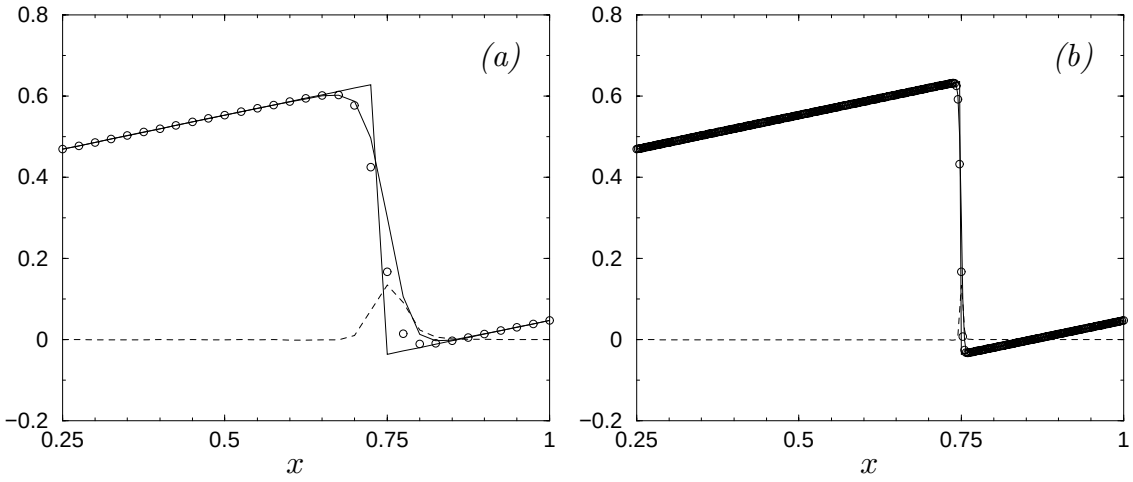

FIGURE 2. Solution for Burger's equation at $t = 2.5$, $N = 80$; (a) with DDM: —— $\bar{u}$, —— u_{ex}, ∘ $\bar{u}_{ex}$, - - - - $(\overline{u}_{ex} - \overline{u})$; (b) with $N = 800$; note that the domain has been truncated for clarity.

the term vanishes asymptotically:

$$\lim_{\xi \to \infty} \|I - G_2\| = 0 \ .$$

These properties ensure that (5) is consistent with (1). It remains to show that (4) provides sufficient numerical-entropy dissipation by consistency with the entropy condition

$$\frac{\partial \eta(u)}{\partial t} + \frac{\partial \psi(u)}{\partial x} \leq 0$$

where $\eta(u)$ and $\psi(u)$ is a convex entropy pair (Lax 1973). By condition (15) it is obvious that the relaxation term provides entropy dissipation for $\chi > 0$:

$$(\bar{u}, (I - G_2) * \bar{u}) = (\bar{u}, \bar{u}) - (\bar{u}, G_2 * \bar{u}) \geq (\bar{u}, \bar{u})(1 - \|G_2\|) \geq 0$$

using $\|G_2\| \leq 1$, where $(\cdot, \cdot)$ is a suitable inner product and $\|\cdot\|$ the corresponding norm. The amount of entropy dissipation is controlled by choosing G_2 and the relaxation constant χ. The determination of χ from an entropy condition is subject to ongoing work.

2.3 Example: Inviscid Burger's equation

For numerical discretization a 6th order symmetric compact finite-difference scheme is used (Lele, 1992). At interior mesh points the difference operator for a grid function $f_i = f(x_i)$ is given by

$$f'_{i-1} + 3f'_i + f'_{i+1} = \frac{1}{h}(-\frac{1}{12}f_{i-2} - \frac{7}{3}f_{i-1} + \frac{7}{3}f_{i+1} + \frac{1}{12}f_{i+2}) \ . \qquad (16)$$

We found that this scheme gives for all test cases better results than a second order central finite-difference scheme. Time integration is performed with an explicit 3rd order Runge-Kutta scheme.

The variable u of Eq. (1) is a scalar, and the flux function is $F(u) = u^2/2$. The solution u is 2-periodic, and the initial condition is given by $u_0(x) = 0.3 - 0.7\sin(\pi x)$, $-1 \leq x < 1$. The domain is discretized into N evenly spaced subintervals. The relaxation constant is set $\chi = 1/h$, where h is the grid spacing. Due to the relaxation term, the time-step size τ for the explicit time-integration is reduced. Stable integration is achieved with a CFL-number of $CFL = 0.5$. Note, however, that this restriction may be circumvented either by using a semi-implicit time-integration (the relaxation term is linear in the solution) or by recognizing that the relaxation term can be implemented by using the secondary filtering every $(1/\chi)/\tau$ time-steps. The latter corresponds to a time-split discretization of the regularized transport equation (Adams, 1999). Figure 2 shows the results obtained at time $t = 2.5$ for 80 and 800 grid points.

3. Future plans

The determination of the relaxation constant χ using numerical-entropy considerations is presently in progress. The scheme has been successfully applied also to the one-dimensional Euler equations and the 'slow-shock problem' (see Adams & Leonard, 1999, Adams, 1999). Tests and applications for two and three dimensions are planned for the near future.

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