A Higher Order Modified Godunov's Method for PDE's with Stiff Sources

Miniati & Colella 2007, JCP, 224, 519; Miniati & Colella 2009, JCP, in prep.

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Definitions

Cons. Eq.

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = S(U)$$

Stiffness

$$\frac{\max\left(\left|\lambda_k\right|\right)}{\min\left(\left|\lambda_k\right|\right)} \gg 1$$

Source term: diffusion, relaxation, endothermic, drag...

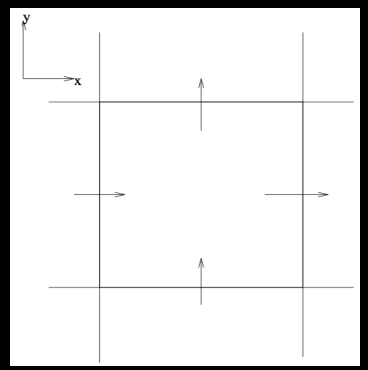
Non-stiff regime

$$U^{n+1} = U^n - \frac{\Delta t}{\Delta x}\left(\Delta F\right)^{n+\frac{1}{2}} + \frac{\Delta t}{2}\left(S\left(U^n\right) + S\left(U^{n+1}\right)\right)$$

Predictor
Primitive
formulation

$$\frac{\partial W}{\partial t} + A\frac{\partial W}{\partial x} = S(W),$$

$$A \equiv \frac{\partial W}{\partial U}\frac{\partial F}{\partial U}\frac{\partial U}{\partial W} = uI + A_L$$



$$W_{\pm} = W_i^n + \frac{1}{2}\left(I - \frac{\Delta t}{\Delta x}A\right)\sum_{\pm\lambda_k > 0}\left(l_k \cdot \Delta W\right) r_k$$

$$W_{\pm} = W_{\pm} + \frac{\Delta t}{2}S\left(W_i^n\right)$$

Hydrodynamics $U = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \; W = \begin{pmatrix} \rho \\ u \\ P \end{pmatrix}, \; F = \begin{pmatrix} \rho u \\ \rho u^2 \\ (\rho E + P)u \end{pmatrix}$

Fractional Step Method

$$\frac{\partial U}{\partial t} = -\nabla \cdot F(U) \equiv H \cdot U$$

$$\frac{dU}{dt} = S(U) \qquad \equiv \Sigma \cdot U$$

$$U(t + 2\Delta t) = \Sigma_{\Delta t/2} H_{\Delta t} \Sigma_{\Delta t} H_{\Delta t} \Sigma_{\Delta t/2}$$

Operator splitting (Strang 1968, LeVeque 1997) provides only first order accuracy (Pember 1984).

Extensive literature on the issue (Chen et al 1994, Jin1995, Jin & Levermore 1996, Caflish et al. 1997, Jin et al 1998) mostly RK+MoL, more recently Dumbser et al (2008) ADER framework.

Our proposal

- Modified predictor step to account for the effect of source term on the hyperbolic structure of the system.
- Apply a one step, 2nd order, A- and L-stable integrator to the ODE (SDC by Dutt, Greengard & Rokhlin 2000; α-QSS by Mott, Oren & van Leer 2000).

$$\frac{dU}{dt} = S(U) - (\nabla \cdot F)^{n+\frac{1}{2}}$$

Lagrangean Trajectories

$$\frac{DW}{Dt} = -A_L \frac{\partial W}{\partial x} + S(W) \simeq -A_L \frac{\partial W}{\partial x} + S(W_0) + \frac{\partial S}{\partial W} \cdot \left(W - W_0\right)$$

Duhamel's formula:

$$W(t) = W_0 + \int_0^t e^{(t-\tau)\,\partial S/\partial W} \left(-A_L \frac{\partial W}{\partial x} + S\left(W_0\right) \right) d\tau$$

$$\simeq W_0 + \left[\frac{1}{t} \int_0^t e^{(t-\tau)\,\partial S/\partial W}\, d\tau \right] \cdot \left(-A_L \frac{\partial W}{\partial x} + S\left(W_0\right) \right) t$$

$$\equiv \Im_{\partial S/\partial W}(t) \cdot \left(-A_L \frac{\partial W}{\partial x} + S\left(W_0\right) \right) t$$

Modified Dynamics

$$\frac{DW}{Dt} + \Im_{(\partial S/\partial W)_0}(t) \cdot A_L \frac{\partial W}{\partial x} = \Im_{(\partial S/\partial W)_0}(t) \cdot S\left(W_0\right)$$

- The operator '$\Im$' tends to the identity as the eigenvalues of '∂S/∂W' become small compared to 't', thus recovering the usual system in primitive form.
- In the opposite limit, however, the operator '$\Im$' projects out the stiff dynamics, leaving only processes resolved over a timestep t, and effectively enforcing the equilibrium EoS.

Modified Predictor Step

$$W_{\pm} = W_i^n + \frac{1}{2}\left[I - \frac{\Delta t}{\Delta x}\left(\Im_{(\partial S/\partial W)_0}\left(\Delta t/2\right)\cdot A_L + uI \right)\right] \sum_{\pm\lambda_k > 0} \left(l_k \cdot \Delta W \right) r_k$$

$$W_{\pm} = W_{\pm} + \frac{\Delta t}{2} \Im_{(\partial S/\partial W)_0}\left(\Delta t/2\right)\cdot S\left(W_i^n\right)$$

$$\Im_{\partial S/\partial W}(t) \equiv \frac{1}{t}\int_0^t e^{(t-\tau)\,\partial S/\partial W}\, d\tau$$

The characteristic analysis is now carried out on the operator '$\Im \cdot A_L$', and both characteristic tracing and Riemann solver are based on the hyperbolic structure of this operator.

Applications

- Endothermic processes (energy sources)
- Dust drag (momentum)
- Radiation Hydrodynamics (M. Sekora & J. Stone)

Endothermic Processes

$$S(W) = (0,0,\Lambda)^T,\ \Lambda \equiv \frac{de}{dt}, \quad e.g.\ \Lambda(e) = K(e - e_{Eq}),$$

$$\Lambda_e \equiv \frac{\partial \Lambda}{\partial e} \neq 0, \quad \Lambda_\rho \equiv \frac{\partial \Lambda}{\partial \rho} = 0$$

$$c \to c_{eff} = \left\{ \left[\alpha(\gamma - 1) + 1 \right] \frac{P}{\rho} \right\}^{1/2}$$

$$\alpha \equiv \frac{e^{\Lambda_e \Delta t/2} - 1}{\Lambda_e \Delta t / 2}, \quad 0 < \alpha \leq 1$$

$$c_{eff} = \begin{cases} \sqrt{\gamma P / \rho} & \text{for } \alpha \to 1 \ \text{(non-stiff)} \\ \sqrt{P / \rho} & \text{for } \alpha \to 0 \qquad \text{(stiff)} \end{cases}$$

Convergence Rates

Table 3
Convergence rates: 2-D case: $A = 10^{-2}$, $\mathbf{k} = (2/\sqrt{5}, 1/\sqrt{5})$

N_{cell}	Density				Momentum			
	L_1	L_2	L_∞	R_1[a]	L_1	L_2	L_∞	R_1[a]
$K = 1$								
32	3.2E−5	3.5E−5	5.3E−5	–	4.3E−5	4.8E−5	7.0E−5	–
64	8.6E−6	9.5E−6	1.4E−5	1.9	9.8E−6	1.1E−5	1.6E−5	2.1
128	2.2E−6	2.5E−6	3.6E−6	2.0	2.3E−6	2.6E−6	3.8E−6	2.1
256	5.7E−7	6.4E−7	9.2E−7	2.0	5.7E−7	6.3E−7	9.1E−7	2.0
$K = 50$								
32	6.2E−5	7.0E−5	1.0E−5	–	3.6E−5	4.0E−5	5.9E−5	–
64	1.2E−5	1.4E−5	2.0E−5	2.4	7.9E−6	8.8E−6	1.3E−5	2.4
128	2.7E−6	3.0E−6	4.3E−6	2.2	1.8E−6	1.9E−6	2.8E−6	2.1
256	6.2E−7	6.9E−7	1.0E−6	2.1	4.0E−7	4.5E−7	6.5E−6	2.2
$K = 10^8$								
32	7.4E−5	8.2E−5	1.2E−4	–	4.5E−5	5.0E−5	7.3E−5	–
64	1.6E−5	1.8E−5	2.6E−5	2.2	1.0E−5	1.1E−5	1.7E−5	2.2
128	3.8E−6	4.2E−6	6.1E−6	2.1	2.5E−6	2.8E−6	4.1E−6	2.0
256	9.4E−7	1.0E−6	1.5E−6	2.0	6.2E−7	6.9E−7	9.9E−6	2.0

[a] R_1 is the convergence rate based on the L_1 errors.

Dust Drag

Velocity equations

$$\frac{du_g}{dx} = -k_g\left(u_g - u_d\right) - \nabla\varphi + \text{hydro terms}$$

$$\frac{dv_d}{dx} = -k_d\left(v_d - u_g\right) - \nabla\varphi$$

Drag coefficients

$$k_g = k_0 \frac{\rho_d}{s} c$$

$$k_d = k_0 \frac{\rho_g}{s} c$$

Stiff conditions either in the limit of small particles sizes (s) and/or high dust densities.

Complications

- want dust as a set of particles, to better represent their collision-less character.
- but stiff regime implies effectively coupling among particles as well.
- So we use with fluid description of dust as an intermediate step to describe gas-dust coupling during the gas update.
- We then advance the particle solution taking into account the drag forces using the gas solution at times ‘t’ and ‘t+Δt’.

Governing Equations

Conservative

$$\frac{\partial U}{\partial t} + \nabla \cdot F = K_U U$$

Primitive

$$\frac{DW}{Dt} = -A_L \frac{\partial W}{\partial x} + K_W W$$

$$U = \begin{pmatrix} \rho_g \\ \rho_g u_g \\ \rho_g E \\ \rho_d \\ \rho_d u_d \end{pmatrix}, \quad W = \begin{pmatrix} \rho_g \\ u_g \\ P \\ \rho_d \\ u_d \end{pmatrix}, \quad F = \begin{pmatrix} \rho_g u_g \\ \rho_g u_g^2 \\ (\rho_g E + P) u_g \\ \rho_d u_d \\ \rho_d u_d^2 \end{pmatrix}$$

Characteristic Speeds

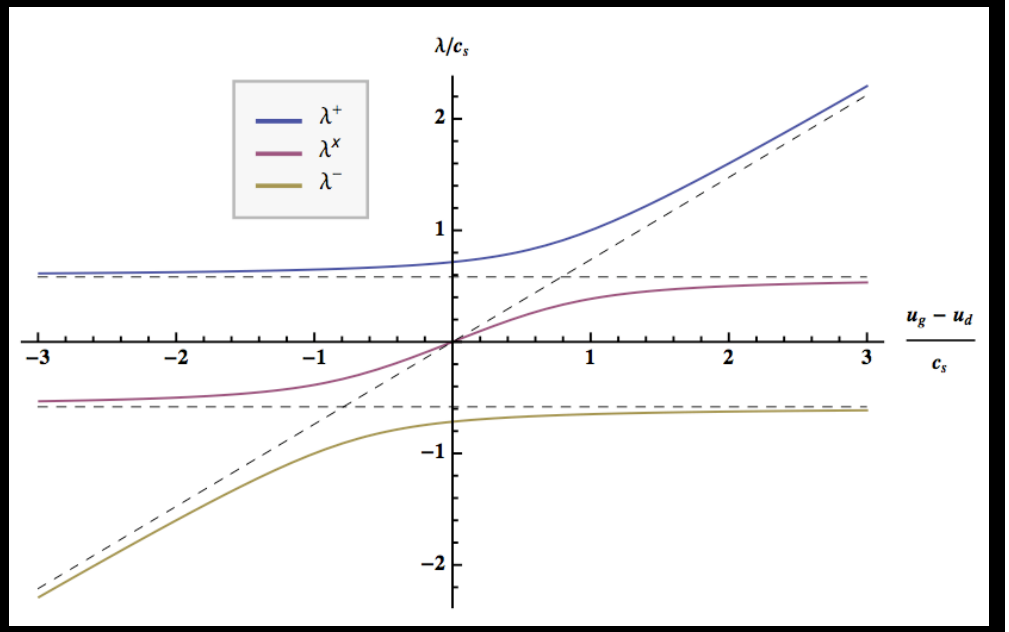
(eigenvalues of the system '$\mathfrak{I} \cdot A_L$')

$$\lambda^0 = 0, \qquad \lambda^d = u_d - u_g$$

$$\lambda^+ = \frac{\hat{\delta u}}{3} + \frac{2}{\sqrt{3}}\left(\hat{c}^2 + \frac{\hat{\delta u}^2}{3}\right)^{1/2} \cos\left(\frac{\varphi}{3}\right)$$

$$\lambda^- = \frac{\hat{\delta u}}{3} + \frac{2}{\sqrt{3}}\left(\hat{c}^2 + \frac{\hat{\delta u}^2}{3}\right)^{1/2} \cos\left(\frac{\varphi}{3} + \frac{2}{3}\pi\right)$$

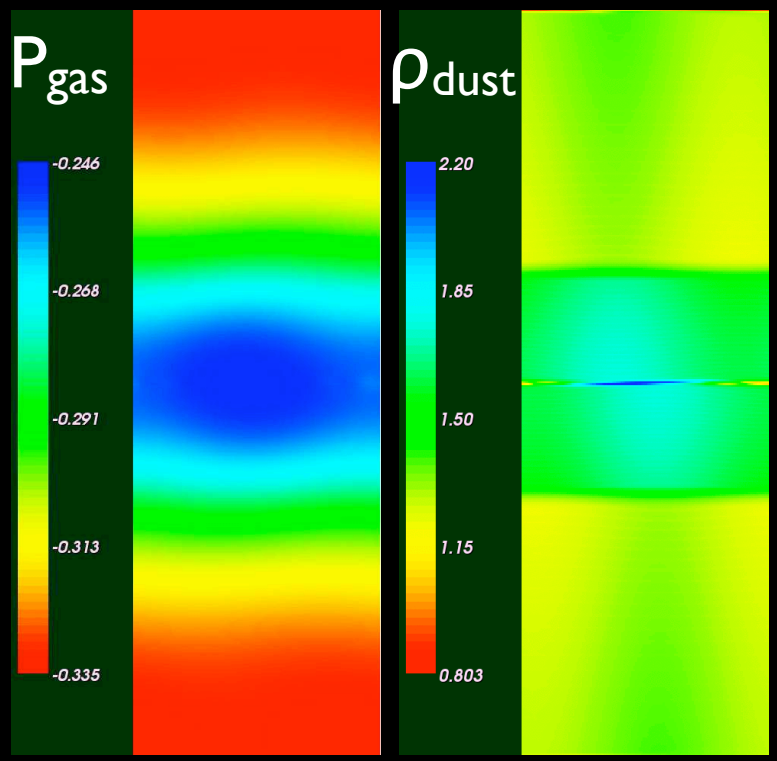
$$\lambda^x = \frac{\hat{\delta u}}{3} + \frac{2}{\sqrt{3}}\left(\hat{c}^2 + \frac{\hat{\delta u}^2}{3}\right)^{1/2} \cos\left(\frac{\varphi}{3} + \frac{4}{3}\pi\right)$$



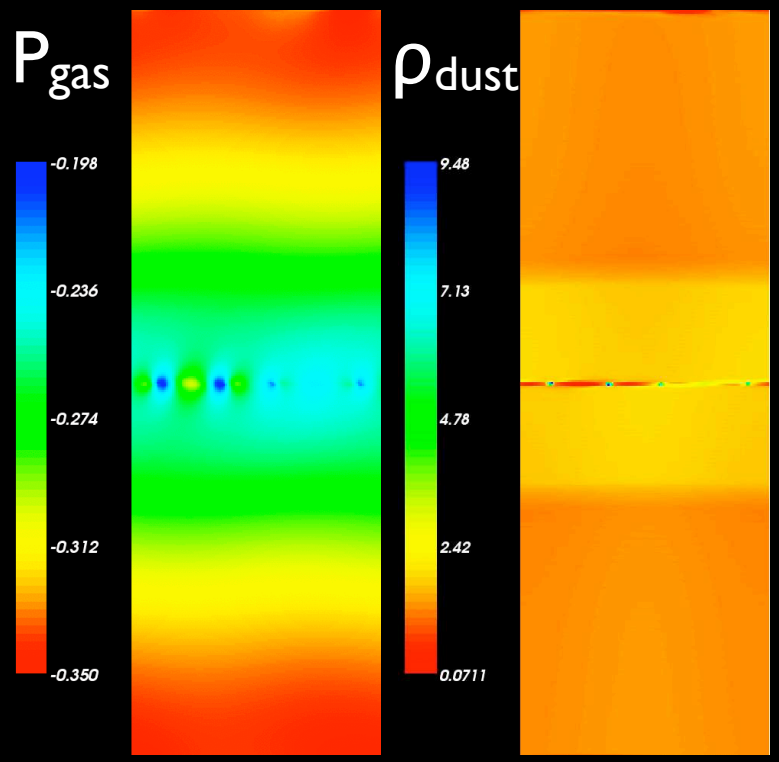
$\hat{\delta u}$ and $\hat{c}$ dust-gas velocity difference modulated by coupling stiffness, φ is a mixing angle between dust driven and acoustic modes, depends on stiffness, ρ_{dust} and ρ_{gas}.

Dust collection at P_{max}

t=0.8



t=1.1



Convergence Rates

Table 7: Convergence Rates: Case D: $A = 1.4 \times 10^{-2}$, $\mathbf{k} = (2,1)/\sqrt{5}$, $\rho_d/\rho_g = 10^2$.

N_{cells}	L_1	R_1	L_2	R_2	L_∞	R_∞	L_1	R_1	L_2	R_2	L_∞	R_∞
	density-gas						**x-vel-gas**					
16	7.5E-06	–	8.4E-06	–	1.2E-05	–	2.3E-04	–	2.6E-04	–	3.6E-04	–
32	2.6E-06	1.5	2.9E-06	1.5	4.2E-06	1.5	1.6E-04	1.5	1.7E-04	1.5	2.5E-04	1.5
64	1.1E-06	1.3	1.2E-06	1.3	1.7E-06	1.3	9.0E-05	1.3	1.0E-04	1.3	1.4E-04	1.3
128	5.8E-07	0.9	6.4E-07	0.9	9.1E-07	0.9	5.4E-05	0.9	5.9E-05	0.9	8.4E-05	0.9
	y-vel-gas						**pressure**					
16	3.2E-04	–	3.5E-04	–	5.0E-04	–	1.1E-05	–	1.2E-05	–	1.7E-05	–
32	2.2E-04	0.5	2.4E-04	0.5	3.4E-04	0.5	3.7E-06	0.5	4.1E-06	0.5	5.8E-06	0.5
64	1.3E-04	0.8	1.4E-04	0.8	2.0E-04	0.8	1.5E-06	0.8	1.7E-06	0.8	2.4E-06	0.8
128	7.2E-05	0.8	8.0E-05	0.8	1.1E-04	0.8	8.1E-07	0.8	9.0E-07	0.8	1.3E-06	0.8
	density-dust						**x-vel-dust**					
16	8.1E-06	–	8.9E-06	–	1.2E-05	–	4.4E-04	–	4.8E-04	–	6.8E-04	–
32	3.2E-06	1.3	3.6E-06	1.3	5.1E-06	1.3	2.2E-04	1.3	2.5E-04	1.3	3.5E-04	1.3
64	1.3E-06	1.3	1.5E-06	1.3	2.1E-06	1.3	1.1E-04	1.3	1.2E-04	1.3	1.7E-04	1.3
128	6.4E-07	1.0	7.1E-07	1.0	1.0E-06	1.0	5.8E-05	1.0	6.5E-05	1.0	9.2E-05	1.0
	y-vel-dust											
16	6.1E-04	–	6.8E-04	–	9.5E-04	–						
32	3.1E-04	1.0	3.4E-04	1.0	4.9E-04	1.0						
64	1.5E-04	1.0	1.7E-04	1.0	2.4E-04	1.0						
128	7.9E-05	1.0	8.8E-05	1.0	1.2E-04	1.0						

Table 5: Convergence Rates: Case B: $\kappa_0 = 10^6$, $\mathbf{k} = (2,1)/\sqrt{5}$, $\rho_d/\rho_g = 1$.

N_{cells}	L_1	R_1	L_2	R_2	L_∞	R_∞	L_1	R_1	L_2	R_2	L_∞	R_∞
	density-gas						**x-vel-gas**					
16	1.9E-4	–	2.1E-4	–	3.1E-4	–	8.6E-5	–	9.4E-5	–	1.5E-4	–
32	8.3E-5	1.2	9.2E-5	1.2	1.4E-4	1.2	3.0E-5	1.2	3.4E-5	1.2	6.0E-5	1.2
64	3.9E-5	1.1	4.3E-5	1.1	6.6E-5	1.1	1.9E-5	1.1	2.1E-5	1.1	3.6E-5	1.1
128	2.0E-5	1.0	2.2E-5	1.0	3.3E-5	1.0	8.6E-6	1.0	9.5E-6	1.0	1.7E-5	1.0
	y-vel-gas						**pressure**					
16	1.4E-4	–	1.6E-4	–	2.4E-4	–	2.7E-4	–	3.0E-4	–	4.3E-4	–
32	5.1E-5	1.5	5.7E-5	1.5	8.8E-5	1.4	1.2E-4	1.5	1.3E-4	1.5	1.9E-4	1.4
64	3.4E-5	0.6	3.8E-5	0.6	5.6E-5	0.7	5.5E-5	0.6	6.1E-5	0.6	9.2E-5	0.7
128	2.1E-5	0.7	2.4E-5	0.7	3.4E-5	0.7	2.7E-5	0.7	3.0E-5	0.7	4.7E-5	0.7
	density-dust						**x-vel-dust**					
16	1.1E-4	–	1.3E-4	–	1.8E-4	–	7.3E-5	–	8.1E-5	–	1.2E-4	–
32	4.8E-5	1.2	5.3E-5	1.2	8.3E-5	1.2	1.0E-5	1.2	1.1E-5	1.2	2.0E-5	1.2
64	2.1E-5	1.2	2.4E-5	1.1	3.9E-5	1.1	2.8E-6	1.2	3.2E-6	1.1	6.4E-6	1.1
128	1.0E-5	1.1	1.1E-5	1.1	1.8E-5	1.1	1.0E-6	1.1	1.4E-6	1.1	5.3E-6	1.1
	y-vel-dust											
16	2.4E-4	–	2.7E-4	–	3.9E-4	–						
32	1.3E-4	0.9	1.5E-4	0.9	2.1E-4	0.9						
64	6.3E-5	1.0	7.0E-5	1.1	1.0E-4	1.0						
128	3.1E-5	1.0	3.4E-5	1.0	4.8E-5	1.1						

Summary

- We have presented a higher order Godunov's method for conservation equations with stiff source terms.
- The novelty of the method consist in the formulation of a modified predictor step derived from a local effective dynamics based on Duhamel's formula.
- For a relaxation law describing endothermic procs., the method is shown to be second order accurate independent of the stiffness conditions.
- A hybrid particle-gas system stiffly coupled through momentum exchange (via drag) is stable and first order accurate.