Finite Volume/DG Schemes Based on Constrained Minimization Function Recovery

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London Mathematical Society Durham Symposium Computational Linear Algebra for Partial Differential Equations JULY 15, 2008



+ Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.



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The Equations of Gas Dynamics







Lagrangian Coordinates

Let

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}, t), \quad \mathbf{x} = (x_i) \in \mathbb{R}^d, \ d = 2 \text{ or } 3,$$

with initial condition

$$\mathbf{x}\big|_{t=0} = \boldsymbol{\xi}.$$

By definition, the pair $(\boldsymbol{\xi}, t)$ is called Lagrangian coordinates associated with the velocity field v. Let

$$J(\boldsymbol{\xi}, t) = \det \left(\frac{\partial x_i(\boldsymbol{\xi}, t)}{\partial \xi_j} \right).$$

Define, $\overline{\varphi}(\boldsymbol{\xi}, t) = \varphi(\mathbf{x}(\boldsymbol{\xi}, t), t)$. Then

$$\frac{\partial \left(\overline{\varphi}J\right)}{\partial t} = J\left(\frac{\overline{\partial\varphi}}{\partial t} + \overline{\operatorname{\mathbf{div}}\ \left(\varphi\ \mathbf{v}\right)}\right).$$







Integral Form of Equations

Conservation of mass:

$$\frac{\partial}{\partial t} \int_{V(t)} \varrho \, d \, \mathbf{x} = 0.$$

Conservation of momentum:

$$\frac{\partial}{\partial t} \int_{V(t)} \varrho \mathbf{v} \ d \ \mathbf{x} = -\int_{V(t)} \nabla p \ d \ \mathbf{x}.$$

Conservation of total energy:

$$\frac{\partial}{\partial t} \int\limits_{V(t)} \varrho \ E \ d\mathbf{x} = - \int\limits_{V(t)} \mathbf{div} \ \left(p \ \mathbf{v} \right) \ d\mathbf{x}.$$





Conservation of Momentum: a General Integral Form

Let
$$\mathbf{x}^{\underline{\alpha}} = x_1^{\alpha_1} \dots x_d^{\alpha_d}$$
. Then
 $\frac{\partial}{\partial t} \int_{V(t)} \rho \, \mathbf{x}^{\underline{\alpha}} \mathbf{v} \, d \, \mathbf{x} = -\int_{V(t)} \mathbf{x}^{\underline{\alpha}} \, \nabla p \, d \, \mathbf{x}.$

Proof:

$$\begin{split} \frac{\partial}{\partial t} \int\limits_{V(t)} \mathbf{x}^{\underline{\alpha}} \, \varrho \mathbf{v} \, d \, \mathbf{x} &= \frac{\partial}{\partial t} \int\limits_{V(0)} \boldsymbol{\xi}^{\underline{\alpha}} \, \overline{\varrho \mathbf{v}} \, J \, d \, \boldsymbol{\xi} \\ &= \int\limits_{V(0)} \boldsymbol{\xi}^{\underline{\alpha}} \, \frac{\partial \, \overline{\varrho \mathbf{v}} \, J}{\partial t} \, d \, \boldsymbol{\xi} \\ &= \int\limits_{V(t)} \mathbf{x}^{\underline{\alpha}} \, \left(\sum_{j=1}^{d} \frac{\partial \varrho v_{j} \, \mathbf{v}}{\partial x_{j}} + \frac{\partial \varrho \mathbf{v}}{\partial t} \right) \, d \, \mathbf{x} \\ &= -\int\limits_{V(t)} \mathbf{x}^{\underline{\alpha}} \, \nabla p \, d \, \mathbf{x}. \end{split}$$



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The integral form is the basis for constructing conservative finite volume schemes and also for DG schemes (for $\underline{\alpha} \neq 0$). Consider conservation of momentum equation

$$\frac{\partial}{\partial t} \int_{V(t)} \varrho \mathbf{v} \ d \ \mathbf{x} = -\int_{V(t)} \nabla p \ d \ \mathbf{x}.$$

Use time discretization $t_{n+1} = t_n + \Delta t$ and let $V_n = V(t_n)$. We have, (for an explicit scheme)

$$\frac{1}{\Delta t} \left(\int_{V_{n+1}} \varrho \mathbf{v} \ d \ \mathbf{x} - \int_{V_n} \varrho \mathbf{v} \ d \ \mathbf{x} \right) = - \int_{V_n} \nabla p_h \ d \ \mathbf{x}.$$

Here, p_h is a finite element approximation of p (to be specified).







Let $m(V) = \int_{V} \rho \, d\mathbf{x}$ be the mass associated with a volume *V*. From the conservation of mass equation

$$\frac{\partial}{\partial t} \int_{V(t)} \varrho \ d \ \mathbf{x} = 0,$$

we have that the mass is constant, i.e.,

$$m(V_n) = \int_{V(t_n)} \varrho \, d \, \mathbf{x} = \int_{V(t_{n+1})} \varrho \, d \, \mathbf{x} = m(V_{n+1}).$$

We approximate ρ at $t = t_n$ with discontinuous piecewise constants:

$$\varrho_n = m(V_n)/|V_n| = m(V)/|V_n|.$$





A FV Conservation of Momentum Equation

Then the following FV scheme is straightforward:

$$m(V) \frac{1}{\Delta t} \left(\frac{1}{|V_{n+1}|} \int\limits_{V_{n+1}} \mathbf{v}_{n+1} \, d \, \mathbf{x} - \frac{1}{|V_n|} \int\limits_{V_n} \mathbf{v}_n \, d \, \mathbf{x} \right) = -\int\limits_{V_n} \nabla p_h \, d \, \mathbf{x}.$$

It is clear that we can compute the average values

$$\frac{1}{|V_{n+1}|} \int_{V_{n+1}} \mathbf{v}_{n+1} \ d \ \mathbf{x} = \frac{1}{m(V)} \int_{V_{n+1}} \varrho \ \mathbf{v}_{n+1} \ d \mathbf{x},$$

without knowing the actual approximation v_h to v_{n+1} .







Thus the problem of function recovery arises: Given the (weighted) average values

$$\frac{1}{m(V)} \int_{V_{n+1}} \varrho \mathbf{v}_{n+1} \ d \mathbf{x},$$

construct a smooth function v_h (that has the prescribed averages) to be used in the approximation of conservation of energy equation

$$\frac{1}{\Delta t} \left(\int_{V_{n+1}} \varrho \varepsilon \, d\mathbf{x} - \int_{V_n} \varrho \varepsilon \, d\mathbf{x} \right) = - \int_{V_{n+1}} p_h \, \mathbf{div} \, \mathbf{v}_h \, d\mathbf{x}.$$

We formulate one function recovery procedure based on minimizing certain energy functional subject to some constraints.







Constrained Total Variation (TV) Function Recovery

We need a second finite element mesh T_h , a refinement of the primal (FV or finite element) mesh T_H .

The accuracy of the scheme is determined by T_H .

The TV function recovery reads:

Find a finite element function \mathbf{v}_h with minimal total variation

$$\mathbf{J}_{TV}(\mathbf{v}_h) = \int_{\Omega} |\nabla \mathbf{v}_h| \ d\mathbf{x} \mapsto \min,$$

with prescribed integral moments for all $V = V_{n+1} \in \mathcal{T}_H$

$$\int_{V} \varrho \mathbf{v}_h \, d\mathbf{x}$$







Constrained Total Variation (TV) Function Recovery

Consider now the conservation of energy equation (for *V* as an union of elements from T_h):

$$\int_{V_{n+1}} \varrho_{n+1} E_{n+1} \, d\mathbf{x} = \int_{V_n} \varrho_n E_n \, d\mathbf{x}_n - \Delta t \, \int_{\partial V_{n+1}} p_h \mathbf{v}_h \cdot \mathbf{n} \, d\sigma.$$

From physical consideration (nonnegative internal energy), splitting $E = \varepsilon + \frac{1}{2} |\mathbf{v}|^2$, gives

$$0 \leq \left(\int_{V_{n+1}} \varrho \varepsilon \, d\mathbf{x} = \right) \int_{V_n} \varrho_n E_n \, d\mathbf{x}_n - \Delta t \int_{\partial V_{n+1}} p_h \mathbf{v}_h \cdot \mathbf{n} \, d\sigma - \frac{1}{2} \int_{V_{n+1}} \varrho_{n+1} \, |\mathbf{v}_h|^2 \, d\mathbf{x}.$$

This is a quadratic inequality constraint for $\mathbf{v}_h = \mathbf{v}_{n+1}$ imposed on any $V = V_{n+1} \in \mathcal{T}_H$ (viewed as a fine-grid, \mathcal{T}_h , domain), if ϱ_{n+1} and p_h are considered given.







Constrained Energy Minimization Function Recovery

Similar problem can be formulated for p_h . Find a finite element function p_h such that

$$J_{TV}(p_h) = \int_{\Omega} |\nabla p_h| \, d\mathbf{x} \mapsto \min,$$

subject to the equality constraints (for all $V \in T_H$) using the E.O.S.:

$$\frac{1}{|V|} \int_{V} p_h \, d\mathbf{x} = \overline{p} \equiv \frac{\gamma - 1}{|V|} \int_{V} \varrho \varepsilon \, d\mathbf{x}.$$

Note that the quadratic inequality for \mathbf{v}_h implies that $\overline{p} \ge 0$.







The equality constraints can be imposed (approximately) via the Rudin-Osher-Fatemi noise removal functional (Physica D, 1992):

$$J_{ROF}(p_h) = \|p_h - \overline{p}\|_0^2 + \epsilon \int_{\Omega} |\nabla p_h| \, d\mathbf{x} \mapsto \min.$$

The purpose of the recovery procedure is to construct a smooth function (with prescribed averages) so that its derivatives (grad and/or div) can be used to close-up the overall FV/DG scheme. That is,

- we first have a sort of "interpolation" procedure (from averages construct a function), and then
- perform "numerical differentiation" (use grad or div).

This is an **ill–posed** problem. Hence the need of **regularization**, which is provided by the TV-functional.





Non-oscillatory TV Function Recovery









We have a primal (moving) mesh T_H . In the recovery procedures, we need a dynamically constructed mesh T_h that is a refinement of T_H . Algorithm 1 (Conservative FV scheme)

To move the mesh, find a finite element function \mathbf{x}_h such that

$$\|\mathbf{x}_h - (\mathbf{x}_n + \Delta t \mathbf{v}_n)\|_0^2 + \epsilon \int_{\Omega_n} |\nabla \mathbf{x}_h| \mapsto \min.$$

Then, \mathbf{x}_{n+1} equals \mathbf{x}_h restricted to the vertices of \mathcal{T}_H (at $t = t_n$) and defines the vertices of the moved \mathcal{T}_H at time $t = t_{n+1}$. Thus, we can compute the volumes |V| for any $V = V_{n+1} \in \mathcal{T}_H$. We can then compute

$$\varrho_{n+1} = \frac{m(V)}{|V_{n+1}|}, \qquad \overline{\mathbf{v}}_{n+1} = \frac{1}{m(V)} \begin{bmatrix} \int_{V_n} \varrho_n \mathbf{v}_n \, d\mathbf{x}_n - \Delta t \int_{V_{n+1}} \nabla p_h \, d\mathbf{x}_{n+1} \end{bmatrix}$$







The Overall Scheme

Solve the constrained energy minimization problems for $\mathbf{v}_h \in \mathbf{S}_h$ and $p_h \in S_h$ (vector and scalar H^1 -conforming finite element spaces):

$$\mathbf{J}_{ROF}(\mathbf{v}_h) = \|\mathbf{v}_h - \overline{\mathbf{v}}_{n+1}\|_{0, \ \varrho_{n+1}}^2 + \epsilon \int_{\Omega_{n+1}} |\nabla \mathbf{v}_h| \ d\mathbf{x}_{n+1} \mapsto \min,$$

$$J_{ROF}(p_h) = \|p_h - \overline{p}_{n+1}\|_0^2 + \epsilon \int_{\Omega_{n+1}} |\nabla p_h| \, d\mathbf{x}_{n+1} \mapsto \min,$$

subject to the quadratic inequality constraints for any $V = V_{n+1} \in T_H$

$$-\frac{1}{2}\int_{V_{n+1}} \rho_{n+1} |\mathbf{v}_h|^2 d\mathbf{x} - \Delta t \int_{\partial V_{n+1}} \rho_h \mathbf{v}_h \cdot \mathbf{n} \, d\sigma + \int_{V_n} \rho E_n \, d\mathbf{x}_n \ge 0.$$

From the E.O.S., compute $\overline{p}_{n+1} = \frac{\gamma - 1}{|V_{n+1}|} \int_{V_{n+1}} \varrho_{n+1} \varepsilon_{n+1} d\mathbf{x}_{n+1} = \frac{\gamma - 1}{|V_{n+1}|} \left[\int_{V_n} \varrho_n E_n d\mathbf{x}_n - \Delta t \int_{\partial V_{n+1}} p_h \mathbf{v}_h \cdot \mathbf{n} d\sigma - \frac{1}{2} \int_{V_{n+1}} \varrho_{n+1} |\mathbf{v}_h|^2 d\mathbf{x} \right] \ge 0.$





The nonlinear TV functional is non-elliptic. In practice, we approximate it with a nonlinear elliptic one:

$$|\nabla p_h| \approx \begin{cases} \frac{1}{|\nabla p_h|^2} |\nabla p_h|^2, & \text{if } |\nabla p_h| \ge \delta, \\ \frac{1}{\delta} |\nabla p_h|^2, & \text{if } |\nabla p_h| < \delta, \end{cases} = g_\delta(|\nabla p_h|) |\nabla p_h|^2, \end{cases}$$

for a mesh-dependent tolerance δ . The approximation to the ROF functional gives rise to a quadratic (matrix-vector) functional

$$\mathcal{J}(\mathbf{v}) \equiv \frac{1}{2} \mathbf{v}^T (M + \epsilon A(\mathbf{v})) \mathbf{v} - \mathbf{v}^T \mathbf{b} \mapsto \min.$$

M is the mass-matrix and A comes from the non-linear elliptic form

$$\frac{a(u, \varphi) = \int g_{\delta}(|\nabla u|) \nabla u \cdot \nabla \varphi \, d\mathbf{x}.}{\Omega}$$





The overall minimization procedure is based on monotone Gauss–Seidel iterations within Picard linearization. That is, for a current iterate v we perform a loop over all indices *i*. At every step *i*, based on the unit coordinate vector e_i , we solve 1D quadratic minimization problem:

 $\mathcal{J}(\mathbf{v}+t\mathbf{e}_i)\mapsto\min,\ t\in\mathbb{R},$

subject to the quadratic inequality constraints. The set of constraints provides a set of intervals where $t \in \mathbb{R}$ can vary. All the intervals contain the origin. Thus the intersection of all intervals is non-empty.

In summary, each 1D minimization step involves finding minimum of a (scalar) quadratic functional over a (scalar) interval. This ensures the monotonicity of the process.

One monotone Gauss–Seidel loop is completed after all indices *i* are



visited.



Entropy

Introducing the fluxes

$$\mathbf{f}_{i} = p \begin{bmatrix} 0 \\ \mathbf{e}_{i} \\ 0 \end{bmatrix} + v_{i} \begin{bmatrix} \varrho \\ \varrho \mathbf{v} \\ \varrho E + p \end{bmatrix}, \quad \mathbf{e}_{i} \in \mathbb{R}^{d},$$

the original Euler equations take the vector form

$$\frac{\partial \widehat{\boldsymbol{\eta}}}{\partial t} + \sum_{j=1}^{d} \frac{\partial \mathbf{f}_j}{\partial x_j} = 0.$$

Here $\widehat{\eta} = (\eta_k)_{k=0}^{d+1}$ is the vector of the conserved variables:

$$\eta_0 = \varrho, \boldsymbol{\eta} = (\eta_k)_{k=1}^d = \varrho \mathbf{v}, \text{ and } \eta_{d+1} = \varrho E,$$







Entropy

The E.O.S. gives

$$p = (\gamma - 1)\varrho(E - \frac{1}{2}|\mathbf{v}|^2) = (\gamma - 1)(\eta_{d+1} - \frac{1}{2}|\boldsymbol{\eta}|^2/\eta_0).$$

Thus, in terms of the conserved variables (η_k)

$$\mathbf{f}_{i} = (\gamma - 1)(\eta_{d+1} - \frac{1}{2}|\boldsymbol{\eta}|^{2}/\eta_{0}) \begin{bmatrix} 0\\ \mathbf{e}_{i}\\ 0 \end{bmatrix} + \begin{bmatrix} \eta_{i}\\ \frac{\eta_{i}}{\eta_{0}}\boldsymbol{\eta}\\ \frac{\eta_{i}}{\eta_{0}}\left(\gamma\eta_{d+1} - \frac{\gamma - 1}{2}\frac{|\boldsymbol{\eta}|^{2}}{\eta_{0}}\right) \end{bmatrix}$$







Entropy

The entropy function is

$$U = U(\widehat{\boldsymbol{\eta}}) = U(\eta_0, \boldsymbol{\eta}, \eta_{d+1}) = -\varrho \log \left(\frac{\varepsilon}{\varrho^{\gamma-1}}\right)$$
$$= -\eta_0 \log \left(\frac{\eta_{d+1} - \frac{1}{2} \frac{|\boldsymbol{\eta}|^2}{\eta_0}}{\eta_0^{\gamma}}\right).$$

The entropy fluxes are

$$F_j = Uv_j = U\frac{\eta_j}{\eta_0}.$$

The following relations hold, for any $k = 0, \ldots, d+1$ and $j = 1, \ldots, d$,

$$\nabla_{\widehat{\eta}} U \cdot \frac{\partial \mathbf{f}_j}{\partial \eta_k} = \frac{\partial F_j}{\partial \eta_k}.$$







Entropy Inequality

This property shows that the original (vector) conservation law

$$\frac{\partial \widehat{\boldsymbol{\eta}}}{\partial t} + \sum_{j=1}^{d} \frac{\partial \mathbf{f}_j}{\partial x_j} = 0,$$

implies the (scalar) conservation law (assuming enough smoothness)

$$\frac{\partial U}{\partial t} + \sum_{j=1}^{d} \frac{\partial F_j}{\partial x_j} = 0.$$

Convexity of U and a limit in $\epsilon \mapsto 0$ of an elliptically perturbed system leads to the entropy inequality $(F_j = Uv_j)$

$$\frac{\partial U}{\partial t} + \sum_{j=1}^{d} \frac{\partial (v_j U)}{\partial x_j} = \frac{\partial U}{\partial t} + \operatorname{div} \left(U \mathbf{v} \right) \le 0.$$



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Entropy Inequality

Since $U = -\varrho s$, $s : e^s = \frac{E - \frac{1}{2} |\mathbf{v}|^2}{\varrho^{\gamma - 1}}$, the entropy inequality reads $\frac{\partial (-\varrho s)}{\partial t} + \mathbf{div} \ (-\varrho s \mathbf{v}) \le 0.$

In Lagrangian coordinates, it takes the form:

$$\frac{\partial}{\partial t} \int_{V(t)} \varrho s \ d\mathbf{x} \ge 0.$$

In practice, we can use the inequality (since the mass is constant)

$$\frac{1}{\int_{V_{n+1}} \varrho \, dx} \int_{V_{n+1}} \varrho \, s \, d\mathbf{x} \ge \frac{1}{\int_{V_n} \varrho \, dx} \int_{V_n} \varrho s \, d\mathbf{x}.$$







Discrete Entropy Inequality

That is, the average value of *s* increases:

 $\overline{s}_{n+1} \ge \overline{s}_n.$

We may as well assume that the average value of

$$e^{s} = \frac{E - \frac{1}{2} |\mathbf{v}|^{2}}{\varrho^{\gamma - 1}} = \frac{\varepsilon}{\varrho^{\gamma - 1}}$$

increases. Hence, for the average internal energy $\overline{\varepsilon} = \frac{1}{m(V)} \int_{V} \varrho \varepsilon \, d\mathbf{x}$,

the following discrete entropy inequality holds:

$$\overline{\varepsilon}_{n+1} \ge \left(\frac{\varrho_{n+1}}{\varrho_n}\right)^{\gamma-1} \overline{\varepsilon}_n = \left(\frac{|V_n|}{|V_{n+1}|}\right)^{\gamma-1} \overline{\varepsilon}_n.$$



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Thus in the recovery procedure, we can use the stronger inequality

$$-\frac{1}{2} \int_{V_{n+1}} \varrho_{n+1} |\mathbf{v}_h|^2 d\mathbf{x} - \Delta t \int_{\partial V_{n+1}} p_h \mathbf{v}_h \cdot \mathbf{n} \, d\sigma + \int_{V_n} \varrho_n E_n \, d\mathbf{x}_n$$
$$\left(= \int_{V_{n+1}} \varrho \varepsilon_{n+1} \, d\mathbf{x} \right) \ge \left(\frac{|V_n|}{|V_{n+1}|} \right)^{\gamma-1} \int_{V_n} \varrho_n \varepsilon_n \, d\mathbf{x}.$$

This inequality poses the challenge to find a feasible v_h that satisfies

all the quadratic inequality constraints (for all $V \in T_H$).

Note that the simpler inequalities (with zero on the r.h.s.) are satisfied with $\mathbf{v}_h = 0$.







At t = 0, $p \approx 0$ outside a single volume (square) $V \in T_H$ and p is equal to a constant on V such that the total energy $\int_{\Omega} \rho E \, d\mathbf{x} = 1$. Also, $\mathbf{v} = 0$ and $\rho = 1$ initially. We keep $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial \Omega$ for $t \ge 0$.

The tests show conversion of internal energy into kinetic and vice-versa.









Figure 1: Initial mesh and recovered pressure.



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Figure 12: Moved mesh at time t = 0.0994.









Figure 13: Moved mesh at time t = 0.200.









Figure 14: Moved mesh at time t = 0.289.









Figure 15: Moved mesh at time t = 0.352.









Figure 16: Moved mesh at time t = 0.430.









Figure 17: Moved mesh at time t = 0.534.









Figure 18: Moved mesh at time t = 0.639.









Figure 19: Moved mesh at time t = 0.754.









Figure 20: Moved mesh at time t = 0.857.









Figure 21: Moved mesh at time t = 0.969.







Numerical Illustration: Symmetry



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Conclusions

- We have proposed new conservative fi nite volume schemes (for Lagrangian hydrodynamics).
- They are based on standard integral form of the conservation laws and utilize non-oscillatory (TV based) function recovery.
- The function recovery procedures seem to be able to replace traditionally used "artifi cial viscosity" and limiters.
- The local mesh refi nement used in the function recovery is essential and needs further study for effi ciency. It can easily destroy symmetry.
- The most expensive part in the computation is the constrained minimization with quadratic inequality constraints. To speed it up, we may need a multilevel procedure (not as straightforward due to the quadratic inequalities).
- The monotone Gauss–Seidel in the pressure recovery has provable mesh–independent convergence (there are no inequalities).
- Extension to higher order integral moments is feasible. This will lead to new DG (discontinuous Galerkin) schemes.





