From Finite Volumes to Discontinuous Galerkin and Flux Reconstruction

Sigrun Ortleb

Department of Mathematics and Natural Sciences, University of Kassel

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Numerical simulation of fluid flow

This includes flows of liquids and gases such as flow of air or flow of water.

- Spreading of Tsunami waves (src: NCTR)
- Weather prediction (src: NOAA)
- Flow through sea gates (src: NASA Goddard)

Flow around airplanes (CC BY 3.0

Requirements on numerical solvers:

- High accuracy of computation
- Detailed resolution of physical phenomena
- Stability and efficiency, robustness
- Compliance with physical laws (e.g. conservation)
1. The Finite Volume Method

2. The Discontinuous Galerkin Scheme

3. SBP Operators & Flux Reconstruction

Derivation of fluid equations

Based on

- physical principles: conservation of quantities & balance of forces
- mathematical tools: Reynolds transport & Gauß divergence theorem

Different formulations:

**Integral conservation law**

\[
\frac{d}{dt} \int_V u \, dx + \int_{\partial V} F(u, \nabla u) \cdot n \, d\sigma = \int_V s(u, x, t) \, dx
\]

**Partial differential equation**

\[
\frac{\partial u}{\partial t} + \nabla \cdot F = s
\]

embodies the physical principles
Derivation of the continuity equation

Based on Reynolds transport theorem

\[
\frac{d}{dt} \int_{V_t} u(x, t) \, dx = \int_{V_t} \frac{\partial u(x, t)}{\partial t} \, dx + \int_{\partial V_t} u(x, t) \mathbf{v} \cdot \mathbf{n} \, d\sigma
\]

rate of change in moving volume = rate of change in fixed volume + convective transfer through surface

\((V_t \text{ control volume of fluid particles})\)
Derivation of the continuity equation

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\( (V_t \text{ control volume of fluid particles}) \)

Physical principle: conservation of mass

\[
\frac{dm}{dt} = \frac{d}{dt} \int_{V_t} \rho \, dx = \int_{V_t} \frac{\partial \rho}{\partial t} \, dx + \int_{\partial V_t} \rho \mathbf{v} \cdot \mathbf{n} \, d\sigma = 0
\]
Derivation of the continuity equation

Based on Reynolds transport theorem

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\frac{d}{dt} \int_{V_t} u(x, t) \, dx = \int_{V_t} \frac{\partial u(x, t)}{\partial t} \, dx + \int_{\partial V_t} u(x, t) \, v \cdot n \, d\sigma
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\]

Divergence theorem yields

\[
\int_{V=V_t} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) \right] \, dx = 0 \quad \Rightarrow \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0
\]

continuity equation
The compressible Navier-Stokes equations

... are based on conservation of mass, momentum and energy

\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{s}
\]

\[
\left[ \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F}^{inv} + \nabla \cdot (A(\mathbf{u})\nabla \mathbf{u}) = \mathbf{s} \right]
\]

inviscid & viscous fluxes

Conservative variables \( \mathbf{u} \in \mathbb{R}^5 \), fluxes \( \mathbf{F} \in \mathbb{R}^{3 \times 5} \) and sources \( \mathbf{s} \in \mathbb{R}^5 \)

\[
\mathbf{u} = \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ \rho E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + pl - \tau \\ (\rho E + p)\mathbf{v} - \kappa \nabla T - \tau \cdot \mathbf{v} \end{pmatrix}, \quad \mathbf{s} = \begin{pmatrix} 0 \\ \rho \mathbf{g} \\ \rho (q + \mathbf{g} \cdot \mathbf{v}) \end{pmatrix}
\]

→ simplified programming by representation in same generic form

→ sufficient to develop discretization schemes for generic conservation law
General discretization techniques

Finite differences / differential form
- approximation of nodal values and nodal derivatives
- easy to derive, efficient
- essentially limited to structured meshes

Finite volumes / integral form
- approximation of cell means and integrals
- conservative by construction
- suitable for arbitrary meshes
- difficult to extend to higher order

Finite elements / weak form
- weighted residual formulation
- quite flexible and general
- suitable for arbitrary meshes
Finite volume schemes

... based on the integral rather than the differential form

Integral conservation enforced for small control volumes $V_i$ defined by computational mesh

$$\bar{V} = \bigcup_{i=1}^{K} \bar{V}_i$$

Degrees of freedom: cell means

$$u_i(t) = \frac{1}{|V_i|} \int_{V_i} u(x, t) \, dx$$

To be specified:

- concrete definition of control volumes
- type of approximation inside these
- numerical method for evaluation of integrals and fluxes

cell-centered vs. vertex-centered
possibly staggered for different variables
Why the integral form?

Because this is the form directly obtained from physics.

1D scalar hyperbolic conservation law

\[ f(u) = \frac{1}{2} u^2 \Rightarrow \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \]

(Burgers equation)

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \]

init. cond.: \( u_0(x) = \begin{cases} 
1, & x < 0, \\
\cos(\pi x), & 0 \leq x \leq 1, \\
-1, & x > 1.
\end{cases} \)

PDE theory tells us:

As long as the exact solution is smooth, it is constant along characteristic curves.
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Characteristic curves are straight lines
and cross \( \rightarrow \) smooth solution breaks down
integral form (time integrated) still holds
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Characteristic curves are straight lines and cross \[ \rightarrow \] smooth solution breaks down

integral form (time integrated) still holds

It is important to ensure correct shock speed
Discretization in conservative form

In 1D, the FV scheme can be regarded as a FD scheme *in conservative form*

\[ u_i(t) = \frac{1}{\Delta x_i} \int_{x_{i-1}/2}^{x_{i+1}/2} u(x, t) \, dx \]
Discretization in conservative form

In 1D, the FV scheme can be regarded as a FD scheme *in conservative form*

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    u_i(t) = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t) \, dx
\]

On a control volume \( V = [x_{i-1/2}, x_{i+1/2}] \), the exact solution fulfills

\[
    \frac{d}{dt} \int_{x_{i-1/2}}^{x_{i+1/2}} u \, dx + [f(u)]_{x_{i-1/2}}^{x_{i+1/2}} = 0
\]

discretized:

\[
    \Delta x_i \frac{u_i^{n+1} - u_i^n}{\Delta t} + f(u_{i+1/2}^n) - f(u_{i-1/2}^n) = 0
\]
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\]

flux values \( f(u_{i\pm1/2}) \) depending on unknown face quantities \( u_{i-1/2}, u_{i+1/2} \)
→ reconstruction necessary from available data \( \ldots, u_{i-1}, u_i, u_{i+1}, \ldots \)
→ Introduction of numerical flux functions \( f^* \)

\[
u_i^{n+1} = u_i^n - \frac{\Delta x_i}{\Delta t} \left( f^*(u_i^n, u_{i+1}^n) - f^*(u_{i-1}^n, u_i^n) \right)
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flux values \( f(u_{i\pm 1/2}) \) depending on unknown face quantities \( u_{i-1/2}, u_{i+1/2} \)

→ reconstruction necessary from available data \( \ldots, u_{i-1}, u_i, u_{i+1}, \ldots \)

→ Introduction of numerical flux functions \( f^* \) **The heart of FV schemes**

\[ u_i^{n+1} = u_i^n - \frac{\Delta x_i}{\Delta t} \left( f^*(u_i^n, u_{i+1}^n) - f^*(u_{i-1}^n, u_i^n) \right) \]
Classical numerical flux functions

linked to Riemann problems & characteristic directions

\[
\begin{align*}
\text{Scalar linear equation} & \quad a > 0 \quad (\partial u / \partial t + a \partial u / \partial x) = 0 \\
\text{Linear system of equations} & \quad f^*(u_i, u_{i+1}) = A + u_i + A - u_{i+1} \\
\text{Nonlinear systems} & \Rightarrow \quad f(u) = f^+ + (u) + f^- - (u) \\
\end{align*}
\]

Steger & Warming, van Leer, AUSM and variants
Classical numerical flux functions

linked to Riemann problems & characteristic directions

Upwind methods

Scalar linear equation \( a > 0 \) \( \left( \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \right) \)

\[
\begin{align*}
  u_{i}^{n+1} &= u_{i}^{n} - \frac{\Delta x}{\Delta t} (au_{i}^{n} - au_{i-1}^{n}) \\
  (f^{\ast}(u_{i}, u_{i+1}) &= au_{i})
\end{align*}
\]

Linear system of equations \( \rightarrow f^{\ast}(u_{i}, u_{i+1}) = A^{+}u_{i} + A^{-}u_{i+1} \)

\[
\begin{align*}
  u_{i}^{n+1} &= u_{i}^{n} - \frac{\Delta t}{\Delta x} \left( A^{+}(u_{i}^{n} - u_{i-1}^{n}) + A^{-}(u_{i+1}^{n} - u_{i}^{n}) \right)
\end{align*}
\]

Nonlinear systems \( \rightarrow \text{Flux vector splitting} \)

\[
\begin{align*}
  f(u) &= f^{+}(u) + f^{-}(u) \Rightarrow f^{\ast}(u_{i}, u_{i+1}) = f^{+}(u_{i}) + f^{-}(u_{i+1})
\end{align*}
\]

Steger & Warming, van Leer, AUSM and variants
Roe scheme
exact solution to linear Riemann problem

\[ \frac{\partial \mathbf{u}}{\partial t} + A_{LR}(\mathbf{u}_L, \mathbf{u}_R) \frac{\partial \mathbf{u}}{\partial x} = 0 \]
**Roe scheme**

Exact solution to linear Riemann problem

\[ \frac{\partial u}{\partial t} + A_{LR}(u_L, u_R) \frac{\partial u}{\partial x} = 0 \]

**Properties of Roe matrix** $A_{LR}$

- $A_{LR} \approx A(u) = Df(u)$
- $A_{LR}(u, u) = A(u)$
- $A_{LR}$ is diagonalizable
- $f(u_R) - f(u_L) = A_{LR}(u_R - u_L)$ (mean value property)

Entropy-fix needed
Classical approximate Riemann solvers for Euler equations

Roe scheme

exact solution to linear Riemann problem

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HLL scheme

Godunov-type scheme
Classical approximate Riemann solvers for Euler equations

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entropy-fix needed

HLL scheme

Godunov-type scheme

- approximates only one intermediate state
- based on integral conservation law
What about higher order schemes?
Challenges posed by hyperbolic conservation laws

- Computation of discontinuous solutions (shocks)
- Unphysical oscillations
- Needs additional numerical dissipation
Difficulties regarding discontinuous solutions

Example: Burgers equation

\[ \frac{\partial u}{\partial t} + u \cdot \frac{\partial u}{\partial x} = 0, \quad u(x, 0) = \sin(x) \]

Exact solution

![Exact solution graph]
Difficulties regarding discontinuous solutions

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Exact solution

Projection

Goal: Controll oscillations
A first approach towards higher order

FV schemes with linear reconstruction – modify left and right states

\[ u_{i}^{n+1} = u_{i}^{n} + \frac{\Delta x_{i}}{\Delta t} \left( f^{*}(u_{i}^{n}, u_{i+1}^{n}) - f^{*}(u_{i-1}^{n}, u_{i}^{n}) \right) = 0 \]
A first approach towards higher order

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- linear reconstruction within cells
  \[ u(x) = u_i + s(x - x_i) \]
- preserve integral means
- how to compute slopes \( s \)?
- prevent creation of new max/min
A first approach towards higher order

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enforce TVD property (relates to properties of exact solution)

\[ \sum_i |u_{i+1}^{n+1} - u_i^{n+1}| \leq \sum_i |u_{i+1}^n - u_i^n| \]

sufficient condition

\[ 0 \leq \left\{ \frac{\Delta x s_i}{u_i - u_{i-1}}, \frac{\Delta x s_i}{u_{i+1} - u_i} \right\} \leq 2 \]
A first approach towards higher order

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sufficient condition

\[ 0 \leq \left\{ \frac{\Delta x \cdot s_{i}}{u_{i} - u_{i-1}}, \frac{\Delta x \cdot s_{i}}{u_{i+1} - u_{i}} \right\} \leq 2 \]

Typical example:

\[ s_{i} = \frac{1}{\Delta x} \minmod(u_{i+1} - u_{i}, u_{i} - u_{i-1}) \]

\( \minmod(a, b) = \begin{cases} 0 & |a| \geq |b|, ab \geq 0 \\ a & |a| < |b|, ab > 0 \\ b & |a| \geq |b|, ab > 0 \\ 0 & \text{otherwise} \end{cases} \)
The ENO reconstruction

ENO stands for essentially non-oscillatory

- higher order reconstruction via interpolation
- adaptively choose stencil
- avoid interpolation across shocks
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ENO approach:

- successive increase of polynomial degree via Newton interpolation
- compare divided differences obtained by left or right extension
The ENO reconstruction

ENO stands for *essentially non-oscillatory*

- higher order reconstruction via interpolation
- adaptively choose *stencil*
- avoid interpolation across shocks

ENO approach:

- successive increase of polynomial degree via Newton interpolation
- compare divided differences obtained by left or right extension

ENO properties:

- constructs only one reconstruction polynomial
- prone to round off errors

\[ u_{i-2} \quad u_{i-1} \quad u_i \quad u_{i+1} \quad u_{i+2} \]

\[ x_{i-2} \quad x_{i-1} \quad x_i \quad x_{i+1} \quad x_{i+2} \]
The WENO reconstruction

WENO stands for *weighted essentially non-oscillatory*

- A priori: choice of main (central) stencil as well as secondary stencils
- Compute polynomial reconstruction on *each* stencil, conserve integral means
- Compute weights depending on oscillatory behaviour of reconstruction
- Evaluate weighted sum of reconstruction polynomials
The WENO reconstruction

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- A priori: choice of main (central) stencil as well as secondary stencils
- Compute polynomial reconstruction on *each* stencil, conserve integral means
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- Evaluate weighted sum of reconstruction polynomials

WENO properties:
- The higher the discretization order – the higher the number of required neighbor cells
- Unstructured grids: difficult to construct stencils
- High demand on resources (CPU time / memory requirement)
From Finite Volumes ... 

.. to Discontinuous Galerkin
Discontinuous Galerkin schemes

\[ \frac{d}{dt} \int_{V_i} u_h \Phi \, dx + \int_{\partial V_i} F^*(u_h^-, u_h^+, n) \Phi \, d\sigma - \int_{V_i} F(u_h) \cdot \nabla \Phi \, dx = \int_{V_i} q_h \Phi \, dx \]

- High accuracy & flexibility
- Compact domains of dependance
- Highly adapted to computations in parallel

\( FV: \Phi = \Phi_0 \quad \leftrightarrow \quad DG: \Phi = \Phi_0, \Phi_1, \ldots, \Phi_N \)

→ Closer link to given physical equations
High resolution of DG scheme

Double Mach reflection: Shock hitting fixed wall

Excellent shock resolution & Detailed representation of fine structures

Density distribution: FV vs. DG scheme

Inflow
Outflow
Fixed wall
Initial shock
The triangular grid DG scheme

Hyberbolic conservation law in 2D

\[
\frac{\partial}{\partial t} u(x, t) + \nabla \cdot F(u(x, t)) = 0, \quad (x, t) \in \Omega \times \mathbb{R}^+ 
\]

Initial conditions: \( u(x, 0) = u_0(x) \)
Boundary conditions: inflow/outflow, reflecting walls
The triangular grid DG scheme

Hyperbolic conservation law in 2D

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Boundary conditions: inflow/outflow, reflecting walls

Approximation \( u_{h,N}(x, t) \): piecewise polynomial in \( x \), degree \( \leq N \)

\( \mathcal{T}^h = \{ \tau_1, \tau_2, \ldots, \tau_{\#T^h} \} \)

Triangulation
The triangular grid DG scheme

Multiplication by test functions $\Phi \in \mathcal{P}^N(\tau_i)$, Integration over $\tau_i$

$$\frac{d}{dt} \int_{\tau_i} u \Phi \, dx + \int_{\tau_i} \nabla \cdot F(u) \, \Phi \, dx = 0$$

Use divergence theorem

$$\frac{d}{dt} \int_{\tau_i} u \Phi \, dx + \int_{\partial \tau_i} F(u) \cdot n \, \Phi \, d\sigma - \int_{\tau_i} F(u) \cdot \nabla \Phi \, dx = 0$$
The triangular grid DG scheme

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$u_{h,N}$  $F^*(u_{h,N}^-, u_{h,N}^+, n)$  $F(u_{h,N})$
The triangular grid DG scheme

Multiplication by test functions $\Phi \in \mathcal{P}^N(\tau_i)$, Integration over $\tau_i$

$$
\frac{d}{dt} \int_{\tau_i} \mathbf{u} \Phi \, d\mathbf{x} + \int_{\tau_i} \nabla \cdot \mathbf{F}(\mathbf{u}) \, \Phi \, d\mathbf{x} = 0
$$

Use divergence theorem

$$
\frac{d}{dt} \int_{\tau_i} \mathbf{u} \Phi \, d\mathbf{x} + \int_{\partial \tau_i} \mathbf{F}(\mathbf{u}) \cdot \mathbf{n} \, \Phi \, d\sigma - \int_{\tau_i} \mathbf{F}(\mathbf{u}) \cdot \nabla \Phi \, d\mathbf{x} = 0
$$

↑ ↑ ↑

$\mathbf{u}_{h,N}$ $\mathbf{F}^*(\mathbf{u}_{h,N}^{-}, \mathbf{u}_{h,N}^{+}, \mathbf{n})$ $\mathbf{F}(\mathbf{u}_{h,N})$

Use orthogonal polynomial basis $\{\Phi_1, \Phi_2, \ldots, \Phi_{q(N)}\}$ of $\mathcal{P}^N(\tau_i)$

$$
\mathbf{u}_{h,N}|_{\tau_i}(\mathbf{x}, t) = \sum_{k=1}^{q(N)} \hat{u}_k^i(t) \Phi_k(\mathbf{x}), \quad q(N) = (N + 1)(N + 2)/2
$$
Time Evolution of coefficients

\[
\frac{d}{dt} \hat{u}_k^i = \left( -\int_{\partial \Omega_i} F^*(\mathbf{u}_h^-, \mathbf{u}_h^+, \mathbf{n}) \Phi_k d\sigma + \int_{\Omega_i} F(\mathbf{u}_h) \cdot \nabla \Phi_k d\mathbf{x} \right) / \| \Phi_k \|_{L^2}^2
\]

Quadrature rules
With respect to orthogonal basis

Time Evolution of coefficients

\[
\frac{d}{dt} \hat{u}_k^i = \left( -\int_{\partial \tau_i} F^*(u_{h,N}, u_{h,N}^+, n) \Phi_k d\sigma + \int_{\tau_i} F(u_{h,N}) \cdot \nabla \Phi_k dx \right) / \| \Phi_k \|_{L^2}^2
\]

Quadrature rules

→ System of ODEs for coefficients \( \hat{u}_k^i \)

\[
\frac{d}{dt} \hat{U}(t) = \mathcal{L}_{h,N} \left( \hat{U}(t), t \right), \quad \hat{U} = \left[ \hat{u}_k^i \right]_{k=1,\ldots,q(N), i=1,\ldots,\#T^h}
\]
With respect to orthogonal basis

Time Evolution of coefficients

\[
\frac{d}{dt} \hat{u}^i_k = \left( -\int_{\partial \tau_i} F^*(u_{h,N}^-, u_{h,N}^+, n) \Phi_k d\sigma + \int_{\tau_i} F(u_{h,N}) \cdot \nabla \Phi_k dx \right) / \| \Phi_k \|_{L^2}^2
\]

Quadrature rules

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\[
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\]

→ e.g. Runge Kutta time integration

With respect to orthogonal basis

Time Evolution of coefficients

\[
\frac{d}{dt} \hat{u}_k^i = \left( -\int_{\partial \tau_i} F^*(\mathbf{u}_{h, N}^-, \mathbf{u}_{h, N}^+, \mathbf{n}) \Phi_k d\sigma + \int_{\tau_i} F(\mathbf{u}_{h, N}) \cdot \nabla \Phi_k dx \right) / \| \Phi_k \|_{L^2}^2
\]

Quadrature rules

→ System of ODEs for coefficients \( \hat{u}_k^i \)

\[
\frac{d}{dt} \hat{U}(t) = L_{h, N} \left( \hat{U}(t), t \right), \quad \hat{U} = \left[ \hat{u}_k^i \right]_{k=1, \ldots, q(N), i=1, \ldots, \#\mathcal{T}^h}
\]

→ e.g. Runge Kutta time integration


Allows easy incorporation of modal filters Meister, Ortleb, Sonar ’12
Damping strategies for DG

Modify approximate solution

Limiters

- Use neighboring data at shocks
- Often $N = 1$

- Cockburn, Shu ’89
- Krivodonova ’07

(H)WENO-Reconstruction

- Use stencil data
- Weighted interpol. polynomials

- Qiu, Shu ’04/05

Modify equation

Explicit dissipation

$$\frac{\partial u}{\partial t} + \nabla \cdot F(u) = \epsilon \Delta u$$

- In conservation law or discretization
- Time step $O(h^2)$

- Jaffre, Johnson, Szepessy ’95
- Persson, Peraire ’06
- Feistauer, Kučera ’07
Damping for spectral methods

1D periodic case: \[ \frac{\partial}{\partial t} u + \frac{\partial}{\partial x} f(u) = 0, \quad x \in [-\pi, \pi] \]

Fourier method: \[ \frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} P_N f(u_N) = 0 \]
\[ u_N(x, t) = \sum_{|k| \leq N} \hat{u}_k(t) e^{ikx} \]

Modal Filtering

Modify coefficients at times \( t^n \)
\[ u_N^\sigma(x, t^n) = \sum_{|k| \leq N} \sigma \left( \frac{|k|}{N} \right) \hat{u}_k^n e^{ikx} \]

\( \sigma : [0, 1] \rightarrow [0, 1] \)

Gottlieb, Lustman, Orzag '81
Damping for spectral methods

1D periodic case: \[ \frac{\partial}{\partial t} u + \frac{\partial}{\partial x} f(u) = 0, \quad x \in [-\pi, \pi] \]

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Spectral viscosity
Add special viscosity term
\[ \epsilon_N (-1)^{p+1} \frac{\partial^p}{\partial x^p} \left[ Q_N \frac{\partial^p u_N}{\partial x^p} \right] \]

Gottlieb, Lustman, Orzag '81
Tadmor '89
Damping for spectral methods

1D periodic case: \[
\frac{\partial}{\partial t} u + \frac{\partial}{\partial x} f(u) = 0, \quad x \in [-\pi, \pi]
\]

Fourier method:
\[
\frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} \mathcal{P}_N f(u_N) = 0
\]
\[
u_N(x, t) = \sum_{|k| \leq N} \hat{u}_k(t) e^{ikx}
\]

Modal Filtering
Modify coefficients at times \( t^n \)
\[
u_N^\sigma(x, t^n) = \sum_{|k| \leq N} \sigma \left( \frac{|k|}{N} \right) \hat{u}_k^n e^{ikx}
\]
Simple implementation

Spectral viscosity
Add special viscosity term
\[
\epsilon_N (1)^{p+1} \frac{\partial^p}{\partial x^p} \left[ Q_N \frac{\partial^p u_N}{\partial x^p} \right]
\]
Convergence theory, Parameter choice
Shock-density interaction (Shu-Osher test case)

Initial conditions

\[(\rho, v_1, v_2, p) = \begin{cases} (3.857143, 2.629369, 0, 10.333333) & \text{if } x < -4 \\ (1 + 0.2 \cdot \sin(5x), 0, 0, 1) & \text{if } x \geq -4 \end{cases}\]

DG with modal filtering

approximate density solution \((t = 1.8)\)

Discretization: \(N = 5, \ K = 1250\)
Further classical test cases

forward facing step
density $N = 5$, $K = 6496$

double Mach reflection
density $N = 4$, $K = 29312$

shock-vortex interaction
pressure $N = 7$, $K = 2122$
Finite Volumes & Discontinuous Galerkin ...

.. and beyond?
Contents

1. The Finite Volume Method
2. The Discontinuous Galerkin Scheme
3. SBP Operators & Flux Reconstruction
Conservative schemes in 1D

- Finite Volume Method
- Discontinuous Galerkin Method Cockburn/Shu ’89
- Flux Reconstruction Method Huynh ’11
- VCJH Energy Stable FR Method Vincent et al. ’10
- SBP-SAT schemes Originally: Kreiss/Scherer ’74
The 1D DG scheme

Scalar hyperbolic conservation law in 1D

\[ \frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) = 0, \quad t > 0, x \in \Omega = [\alpha, \beta] \]
The 1D DG scheme

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\]

Subdivision of \( \Omega \) in

\[
\Omega = \bigcup_i \Omega_i = \bigcup_i [x_i, x_{i+1}]
\]

approximation of \( u \) on \( \Omega_i \)

\[
u^i_h(x, t) = \sum_{k=1}^{N+1} u^i_k(t) \Phi^i_k(x)
\]

with basis functions \( \Phi^i_k \)

\[
u^i = (u^i_1, \ldots, u^i_{p+1})^T
\]

solution vector

The DG scheme in strong form

\[
\int_{\Omega_i} \frac{\partial u^i_h}{\partial t} \Phi^i_k dx + \int_{\Omega_i} \frac{\partial f^i_h}{\partial x} \Phi^i_k dx = [f^*_i, i - f^i_h(x_i)] \Phi^i_k(x_i) - [f^*_i, i+1 - f^i_h(x_{i+1})] \Phi^i_k(x_{i+1})
\]
The 1D DG scheme

Scalar hyperbolic conservation law in 1D

\[
\frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) = 0, \quad t > 0, \ x \in \Omega = [\alpha, \beta]
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u_i^h(x, t) = \sum_{k=1}^{N+1} u_i^j(t) \phi_i^j(x)
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with basis functions \( \phi_i^j \)

\[
u_i = (u_i^1, \ldots, u_i^{p+1})^T
\]

solution vector

The DG scheme in strong form

\[
\int_{\Omega_i} \frac{\partial u_i^j}{\partial t} \phi_k^i \, dx + \int_{\Omega_i} \frac{\partial f_i^j}{\partial x} \phi_k^i \, dx = \left[ f_{i-1,i}^* - f_h^i(x_i) \right] \phi_k^i(x_i) - \left[ f_{i,i+1}^* - f_h^i(x_{i+1}) \right] \phi_k^i(x_{i+1})
\]

equivalent to

\[
M_{i} \frac{d\nu_i^j}{dt} + S_{i} \phi_i^j = \left[ (f_h - f^*) \phi_i^j \right]_{x_i}^{x_{i+1}}
\]

\[
M_{kl} = \int_{\Omega_i} \phi_k^i \phi_l^i \, dx
\]

\[
S_{kl} = \int_{\Omega_i} \phi_k^i \frac{\partial}{\partial x} \phi_l^i \, dx
\]

\[
\phi_i = (\phi_i^1, \ldots, \phi_i^{p+1})^T
\]
Generalized definition of 1D SBP scheme

Del Rey Fernández et al. ’14

- $\underline{M}$ symmetric positive definite
- $\underline{D} := \underline{M}^{-1} \underline{S}$ approximates $\frac{\partial}{\partial x}$
- $\underline{S} + \underline{S}^T = \underline{B}$ with $(x^\mu)^T \underline{B} x^\nu = (x_{i+1})^{\mu+\nu} - (x_i)^{\mu+\nu}$

SBP mimics integration by parts
Generalized definition of 1D SBP scheme

Del Rey Fernández et al. ’14

- \( M \) symmetric positive definite
- \( D := M^{-1} S \) approximates \( \frac{\partial}{\partial x} \)
- \( S + S^T = B \) with \( (x^\mu)^T B x^\nu = (x_{i+1})^{\mu+\nu} - (x_i)^{\mu+\nu} \)

SBP mimics integration by parts

fulfilled by DG scheme

\[
M \frac{d u}{d t} + S f = \left[(f_h - f^*) \Phi \right]_{x_{i+1}}^{x_i}
\]

- \( M_{kl} = \int_{\Omega_i} \Phi_k \Phi_l \, dx \)
- \( S_{kl} = \int_{\Omega_i} \Phi_k \frac{\partial}{\partial x} \Phi_l \, dx \)
- \( B_{kl} = [\Phi_k \Phi_l]_{x_{i+1}}^{x_i} \)

Gauss-Lobatto (GLL) and Gauss-Legendre (GL) DG schemes:

- \( B_{\text{GLL}} = \text{diag}\{-1, 0, \ldots, 0, 1\} \),
- \( B_{\text{GLL,N=1}} = \text{diag}\{-\sqrt{3}, \sqrt{3}\} \),
- \( B_{\text{GLL,N=2}} = \begin{pmatrix}
  \frac{-1}{\xi^3} & \frac{1-\xi^2}{\xi^3} & 0 \\
  \frac{1-\xi^2}{\xi^3} & 0 & \frac{\xi^2-1}{\xi^3} \\
  0 & \frac{\xi^2-1}{\xi^3} & \frac{1}{\xi^3}
\end{pmatrix} \), \( \xi = \sqrt{\frac{3}{5}} \)
Advantages of SBP schemes

**Provable linear stability**

Energy stability w.r.t. $\frac{1}{2} \| u \|^2_M$
Advantages of SBP schemes

Provable linear stability
Energy stability w.r.t. \( \frac{1}{2} ||u||_{M}^{2} \)

Relation to quadrature formulae
Corresponding QF preserve certain properties of functional
e.g. discrete divergence theorem Hicken/Zingg '13
Advantages of SBP schemes

Provable linear stability
Energy stability w.r.t. $\frac{1}{2} \| u \|_M^2$

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Correct discretization of split form conservation laws

- split forms (e.g. skew-symmetric)
  - $\rightarrow$ Better control of oscillations
  - preservation of secondary quantities, e.g. $\rightarrow$ kinetic energy
Advantages of SBP schemes

**Provable linear stability**
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**Correct discretization of split form conservation laws**
- split forms (e.g. skew-symmetric)
  - \( \rightarrow \) Better control of oscillations
  - preservation of secondary quantities, e.g. \( \rightarrow \) kinetic energy
- possible lack of discrete conservation
Advantages of SBP schemes

**Provable linear stability**
Energy stability w.r.t. $\frac{1}{2} \| u \|_M^2$

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Corresponding QF preserve certain properties of functional
e.g. discrete divergence theorem Hicken/Zingg ’13

**Correct discretization of split form conservation laws**
- split forms (e.g. skew-symmetric)
  - $\rightarrow$ Better control of oscillations
  - preservation of secondary quantities, e.g. $\rightarrow$ kinetic energy
- possible lack of discrete conservation
- SBP schemes: equivalent telescoping form Fisher et al. ’12
  $\rightarrow$ if convergent, then weak solution (Lax-Wendroff)
Observation

Discontinuous Galerkin ↔ Energy Stable Flux Reconstruction (VCJH)
Observation

Discontinuous Galerkin ↔ Energy Stable Flux Reconstruction (VCJH)

These methods meet as SBP schemes!
Spectral difference and flux reconstruction schemes

The SD scheme [Wang et al. '07]

\[
\frac{\partial u}{\partial t} + \frac{\partial f^{SD}}{\partial x} = 0
\]

Construction of \( f^{SD} \)

\[f_{SD} = f_i h + [f^*_{i+1} - f_i h(x_i)] \]

\[f_{CL} g_L \]

\[f_{CR} g_R \]

where \( g_L, g_R \in P_{N+1} \) with

\[g_L(x_i) = 1 \]

\[g_R(x_i) = 0 \]

\[g_L(x_{i+1}) = 0 \]

\[g_R(x_{i+1}) = 1 \]

DG for \( g_L, g_R \) right & left Radau polynomials

In matrix-vector form [Allaneau/Jameson '11]

Expand \( u_h, f_h \) and \( g'_L, g'_R \) in same basis \( \{\Phi_k\} \)

Multiply by \( M \) with

\[M_{kl} = \int_\Omega \Phi_k \Phi_l \, dx\]
Spectral difference and flux reconstruction schemes

The SD scheme [Wang et al. '07]

\[ \frac{\partial u}{\partial t} + \frac{\partial f^{SD}}{\partial x} = 0 \]

Construction of \( f^{SD} \)

Generalized by FR scheme [Huynh '11]

\[ f^{FR} = f_h^i + [f_{i-1,i}^* - f_h^i(x_i)] g_L + [f_{i,i+1}^* - f_h^i(x_{i+1})] g_R \]

where \( g_L, g_R \in P^{N+1} \) with \( \begin{cases} g_L(x_i) = 1 \\ g_L(x_{i+1}) = 0 \\ g_R(x_i) = 0 \\ g_R(x_{i+1}) = 1 \end{cases} \)

DG for \( g_L, g_R \) right & left Radau polynomials
Spectral difference and flux reconstruction schemes

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f^{FR} = f^i_h + [f^{*}_{i-1,i} - f^i_h(x_i)] g_L + [f^{*}_{i,i+1} - f^i_h(x_{i+1})] g_R
\]

where \( g_L, g_R \in P^{N+1} \) with

\[
\begin{align*}
g_L(x_i) &= 1 & g_R(x_i) &= 0 \\
g_L(x_{i+1}) &= 0 & g_R(x_{i+1}) &= 1
\end{align*}
\]

DG for \( g_L, g_R \) right & left Radau polynomials

in matrix-vector form [Allaneau/Jameson ’11]

- expand \( u_h, f_h \) and \( g'_L, g'_R \) in same basis \( \{\Phi_k\} \)
- multiply by \( M \)

with \( M_{kl} = \int_{\Omega_i} \Phi_k \Phi_l \, dx \)

\[
M \frac{du}{dt} + S f = -f_{CL}M g'_L - f_{CR}M g'_R
\]
Spectral difference and flux reconstruction schemes

The SD scheme [Wang et al. '07]

\[ \frac{\partial u}{\partial t} + \frac{\partial f^{SD}}{\partial x} = 0 \]

Construction of \( f^{SD} \)

Generalized by FR scheme [Huynh '11]

\[ f^{FR} = f^i_h + \left[ f^*_{i-1,i} - f^i_h(x_i) \right] g_L + \left[ f^*_{i,i+1} - f^i_h(x_{i+1}) \right] g_R \]

where \( g_L, g_R \in P^{N+1} \) with

\[
\begin{align*}
  g_L(x_i) &= 1 & g_R(x_i) &= 0 \\
  g_L(x_{i+1}) &= 0 & g_R(x_{i+1}) &= 1
\end{align*}
\]

DG for \( g_L, g_R \) right & left Radau polynomials

in matrix-vector form [Allaneau/Jameson '11]

- expand \( u_h, f_h \) and \( g'_L, g'_R \) in same basis \( \{\Phi_k\} \)
- multiply by \( M \)

with \( M_{kl} = \int_{\Omega_i} \Phi_k \Phi_l dx \)

\[
\begin{align*}
  M \frac{du}{dt} + S \, f &= -f_{CL} M g'_L - f_{CR} M g'_R \\
  \left[ \frac{du}{dt} + D \, f \right] &= -f_{CL} g'_L - f_{CR} g'_R, \quad D = M^{-1} S
\end{align*}
\]
Relation of FR framework to DG scheme

Reformulate

\[ M \frac{du}{dt} + Sf = -f_{CL} M g'_L - f_{CR} M g'_R \]

\[ f_{CL} = f_{i-1,i}^* - f_h^i(x_i) \]
\[ f_{CR} = f_{i,i+1}^* - f_h^i(x_{i+1}) \]
Relation of FR framework to DG scheme

Reformulate

\[ M \frac{du}{dt} + Sf = -f_{CL} Mg'_{L} - f_{CR} Mg'_{R} \]

As \( Mg' = \int_{\Omega_i} g' \Phi dx = [g \Phi]_{x_{i+1}}^{x_i} - \int_{\Omega_i} g \Phi' dx \) (\( g' \) is representation of \( g' \))

\[ f_{CL} = f^*_{i-1,i} - f^i_h(x_i) \]
\[ f_{CR} = f^*_{i,i+1} - f^i_h(x_{i+1}) \]
Relation of FR framework to DG scheme

Reformulate

\[ \frac{M}{\partial t} \frac{du}{dt} + Sf = -f_{CL} M g'_L - f_{CR} M g'_R \]

As \( M g' = \int_{\Omega_i} g' \Phi dx = [g \Phi]_{x_i}^{x_{i+1}} - \int_{\Omega_i} g \Phi' dx \) (\( g' \) is representation of \( g' \))

we have \( (\text{as } g_R(x_i) = g_L(x_{i+1}) = 0) \)

\[ RHS_{FR} = f_{CL} \Phi(x_i) - f_{CR} \Phi(x_{i+1}) + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' dx \]

\( RHS_{DG} \) \( \text{Deviation from DG} \)

\( f_{CL} = f_{i-1,i}^* - f_h^i(x_i) \)

\( f_{CR} = f_r^{i,i+1} - f_h^i(x_{i+1}) \)
Relation of FR framework to DG scheme

Reformulate

\[ M \frac{du}{dt} + S f = -f_{CL} M g'_L - f_{CR} M g'_R \]

As \( M g' = \int_{\Omega_i} g' \Phi \, dx = \left[ g \Phi \right]_{x_i}^{x_{i+1}} - \int_{\Omega_i} g \Phi' \, dx \) \( (g' \) is representation of \( g' \))

we have \( (\text{as } g_R(x_i) = g_L(x_{i+1}) = 0) \)

\[ \text{RHS}_{FR} = \underbrace{f_{CL} \Phi(x_i) - f_{CR} \Phi(x_{i+1})}_{\text{RHS}_{DG}} + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' \, dx \]

\( \Rightarrow \) Two equivalent formulations for FR scheme:

\[ M \frac{du}{dt} + S f = \text{RHS}_{DG} + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' \, dx \]

\[ \frac{du}{dt} + D f = -f_{CL} g'_L - f_{CR} g'_R \]
VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

\[
\begin{align*}
M \frac{du}{dt} + S f &= \text{RHS}_{DG} + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' dx \\
K \frac{du}{dt} + K D f &= -f_{CL} K g'_L - f_{CR} K g'_R, \quad K \text{ pos. semidef. with } K D = 0
\end{align*}
\]
VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

\[
M \frac{du}{dt} + S f = \text{RHS}_{DG} + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' dx
\]

\[
K \frac{du}{dt} + K D f = -f_{CL} K g'_L - f_{CR} K g'_R, \quad K \text{ pos. semidef. with } K D = 0
\]

Summing up yields

\[
\left( M + K \right) \frac{du}{dt} + S f = \text{RHS}_{DG} + f_{CL} \left( \int_{\Omega_i} g_L \Phi' dx - K g'_L \right) + f_{CR} \left( \int_{\Omega_i} g_R \Phi' dx - K g'_R \right)
\]
VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

\[
\frac{M}{\text{dt}} \frac{du}{dt} + S f = \text{RHS}_{DG} + \int_{\Omega_i} (f_{CL}g_L + f_{CR}g_R) \Phi' \, dx
\]

\[
K \frac{du}{dt} + KDf = -f_{CL}Kg'_L - f_{CR}Kg'_R, \quad K \text{ pos. semidef. with } K D = 0
\]

Summing up yields

\[
(M + K) \frac{du}{dt} + Sf = \text{RHS}_{DG} + f_{CL} \left( \int_{\Omega_i} g_L \Phi' \, dx - Kg'_L \right) + f_{CR} \left( \int_{\Omega_i} g_R \Phi' \, dx - Kg'_R \right)
\]

VCJH schemes [Vincent/Castonguay/Jameson '10]

- Choose \(g_L, g_R\) such that red terms vanish for suitable \(K\)
VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

\[
\begin{align*}
M \frac{du}{dt} + S f &= \text{RHS}_{DG} + \int_{\Omega_i} (f_{CL}g_L + f_{CR}g_R) \Phi' dx \\
K \frac{du}{dt} + K Df &= -f_{CL}K g_L' - f_{CR}K g_R', \quad K \text{ pos. semidef. with } K D = 0
\end{align*}
\]

Summing up yields

\[
\left( M + K \right) \frac{du}{dt} + S f = \text{RHS}_{DG} + f_{CL} \left( \int_{\Omega_i} g_L \Phi' dx - K g_L' \right) + f_{CR} \left( \int_{\Omega_i} g_R \Phi' dx - K g_R' \right)
\]

VCJH schemes [Vincent/Castonguay/Jameson '10]

- Choose \( g_L, g_R \) such that red terms vanish for suitable \( K \)
- Similar to DG: \( M \leadsto M + K \) (modified mass matrix)
  \( \rightarrow \) “filtered DG scheme” [Allaneau/Jameson '11]
VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

\[
\frac{M}{dt} \frac{du}{dt} + S f = RHS_{DG} + \int_{\Omega_i} (f_{CL} g_L + f_{CR} g_R) \Phi' dx
\]
\[
K \frac{du}{dt} + K D f = -f_{CL} K g_L' - f_{CR} K g_R', \quad K \text{ pos. semidef. with } K D = 0
\]

Summing up yields

\[
(M + K) \frac{du}{dt} + S f = RHS_{DG} + f_{CL} \left( \int_{\Omega_i} g_L \Phi' dx - K g_L' \right) + f_{CR} \left( \int_{\Omega_i} g_R \Phi' dx - K g_R' \right)
\]

VCJH schemes [Vincent/Castonguay/Jameson ’10]

- Choose \( g_L, g_R \) such that red terms vanish for suitable \( K \)
- Similar to DG: \( M \leadsto M + K \) (modified mass matrix)
  \( \to \) “filtered DG scheme” [Allaneau/Jameson ’11]
- Fulfills SBP property! \( D = M^{-1} S = (M + K)^{-1} S \)
Comparison of low order DGSBP schemes

&

Use of kinetic energy preservation and skew-symmetric forms
Smooth solutions to 1D Navier-Stokes equations

Non-linear acoustic pressure wave

\[ \rho(x, 0) = 1, \; \nu(x, 0) = 1, \; p(x, 0) = 1 + 0.1 \sin(2\pi x), \; x \in [0, 1] \]

periodic BC, viscosity \( \mu = 0.002 \), Prandtl number \( Pr = 0.72 \)

**Gauss-Legendre vs. Gauss-Lobatto nodes**

\([N = 1 \text{ on } 80 \text{ cells, KEP flux, } T = 20; \text{ reference: } N = 3 \text{ on } 500 \text{ cells}]\)

Higher accuracy of Gauss-Legendre DG scheme.
2D decaying homogeneous turbulence

Computed on cartesian grid discretizing $\Omega = [0, 2\pi]^2$, periodic b.c.

$T = 1$ \hspace{1cm} $T = 2$ \hspace{1cm} $T = 5$ \hspace{1cm} $T = 10$

$T = 0$: Initial energy spectrum given in Fourier space by

$$E(k) = \frac{a_s}{2} \frac{1}{k_p} \left( \frac{k}{k_p} \right)^{2s+1} \exp \left[ - \left( s + \frac{1}{2} \right) \left( \frac{k}{k_p} \right)^2 \right]$$

for wave number $k = \sqrt{k_x^2 + k_y^2}$ \hspace{1cm} (Parameters $k_p = 12$, $a_s = \frac{74}{48}$)
Energy spectrum $T = 10$

Gauss nodes, $N = 1$

Re=100

SBP operators allow for conservative discretization of fluid equations in skew-symmetric form.
Re=600

Better representation of energy spectrum for KEP scheme. Specifically for in underresolved case.
Current successful implementations of DG and FR schemes
The FLEXI Project

https://www.flexi-project.org


- DG space discretization
- explicit time stepping
- massive scalability
Spectral/hp Element Framework: Nektar++

http://www.nektar.info/gallery/

- CG / DG operators
- hierarchical and nodal expansion bases
- temporal and spatial adaption, MPI parallel communication

DG for OpenFOAM?

http://www.sfb1194.tu-darmstadt.de/teilprojekte_4/b/b05_1/index.de.jsp

- Development within DG framework BoSSS (Bounded Support Spectral Solver)
- To be successively implemented in OpenFOAM

- Level set method for multiphase flow
- High order DG method
- Arbitrarily high accuracy at phase interfaces with cut-cell method

Summary

1. The Finite Volume Method
2. The Discontinuous Galerkin Scheme
3. SBP Operators & Flux Reconstruction
Thank you for your attention!