From Finite Volumes to Discontinuous Galerkin and Flux Reconstruction

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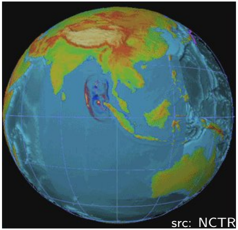
UNIKASSEL VERSITÄT | MATHEMATICS AND NATURAL SCIENCES

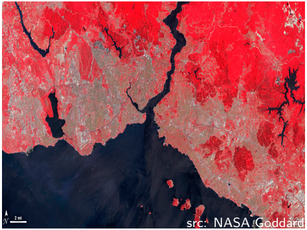
Numerical simulation of fluid flow

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



Spreading of Tsunami waves

Weather prediction



Flow through sea gates

Flow around airplanes

Requirements on numerical solvers

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

Contents

Derivation of fluid equations

Based on

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

Different formulations:

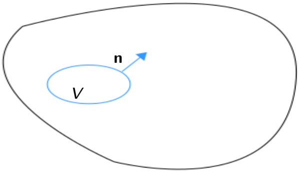
Integral conservation law

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

Partial differential equation

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

embodies the physical principles



Derivation of the continuity equation

Based on Reynolds transport theorem

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

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

(V_t *control volume* of fluid particles)

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Physical principle: conservation of mass

$$\frac{dm}{dt} = \frac{d}{dt}\int_{V_t} \rho\,d\mathbf{x} = \int_{V_t} \frac{\partial \rho}{\partial t} d\mathbf{x} + \int_{\partial V_t} \rho\mathbf{v}\cdot\mathbf{n}\,d\sigma = 0$$

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Divergence theorem yields

$$\int_{V\equiv V_t} \left[\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v})\right] d\mathbf{x} = 0 \quad \Rightarrow \quad \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0$$

continuity equation

The compressible Navier-Stokes equations

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

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

inviscid & viscous fluxes

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

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

convective fluxes,
heat fluxes & surface forces
p pressure, T temperature
τ viscous stress tensor
κ thermal conductivity

body forces
& heat sources
g gravitational & electromag. forces
q intern. heat sources

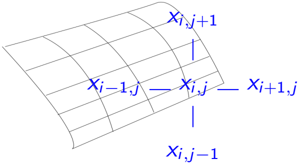
→ simplified programming by representation in same generic form

→ sufficient to develop discretization schemes for generic conservation law

General discretization techniques

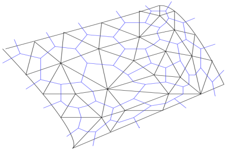
Finite differences / differential form

- approximation of nodal values and nodal derivatives
- easy to derive, efficient
- essentially limited to structured meshes



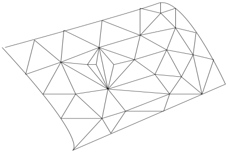
Finite volumes / integral form

- approximation of cell means and integrals
- conservative by construction
- suitable for arbitrary meshes
- difficult to extend to higher order



Finite elements / weak form

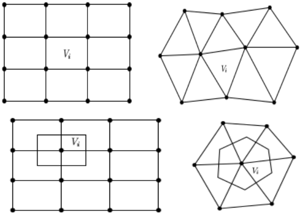
- weighted residual formulation
- quite flexible and general
- suitable for arbitrary meshes



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

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

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



cell-centered vs. vertex-centered

possibly staggered for different variables

Degrees of freedom: cell means

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

To be specified:

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

Why the integral form?

Because this is the form directly obtained from physics.

1D scalar hyperbolic conservation law

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

$f(u)=\frac{1}{2}u^2 \Rightarrow \frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=0$ (Burgers equation)

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

PDE theory tells us:

As long as the exact solution is smooth, it is constant along charactereristic curves

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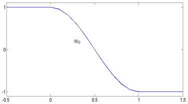

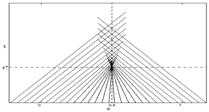

Characteristic curves are straight lines

and cross → smooth solution breaks down

integral form (time integrated) still holds

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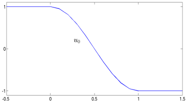

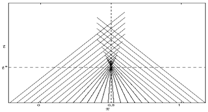

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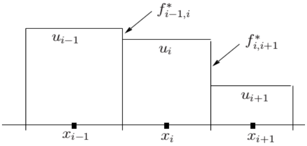
It is important to ensure correct shock speed

Discretization in conservative form

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



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

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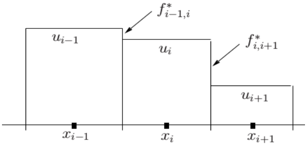

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On a control volume $V = [x_{i-1/2}, x_{i+1/2}]$, the exact solution fulfills

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

discretized: $$\Delta x_i \frac{u_i^{n+1} - u_i^n}{\Delta t} + f(u^n_{i+1/2}) - f(u^n_{i-1/2}) = 0$$

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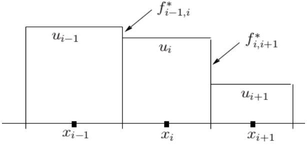

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flux values $f(u_{i\pm 1/2})$ depending on unknown face quantities $u_{i-1/2}, u_{i+1/2}$
$\rightarrow$ reconstruction necessary from available data $\ldots, u_{i-1}, u_i, u_{i+1}, \ldots$

$\rightarrow$ 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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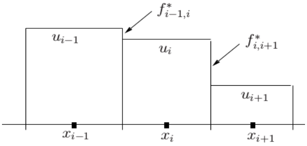

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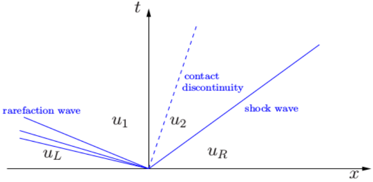
Classical numerical flux functions

linked to Riemann problems
& characteristic directions



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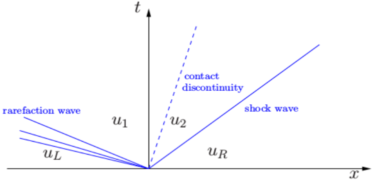


Upwind methods

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

$$u_i^{n+1} = u_i^n - \frac{\Delta x}{\Delta t}\left(au_i^n - au_{i-1}^n\right) \qquad (f^*(u_i, u_{i+1}) = au_i)$$

Linear system of equations $\quad \to \mathbf{f}^*(\mathbf{u}_i, \mathbf{u}_{i+1}) = \mathbf{A}^+\mathbf{u}_i + \mathbf{A}^-\mathbf{u}_{i+1}$

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{A}^+(\mathbf{u}_i^n - \mathbf{u}_{i-1}^n) + \mathbf{A}^-(\mathbf{u}_{i+1}^n - \mathbf{u}_i^n)\right)$$

Nonlinear systems $\quad \to$ Flux vector splitting

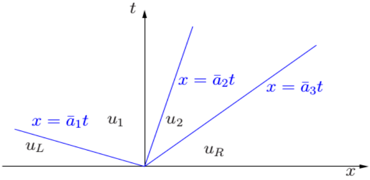
$$\mathbf{f}(\mathbf{u}) = \mathbf{f}^+(\mathbf{u}) + \mathbf{f}^-(\mathbf{u}) \;\Rightarrow\; \mathbf{f}^*(\mathbf{u}_i, \mathbf{u}_{i+1}) = \mathbf{f}^+(\mathbf{u}_i) + \mathbf{f}^-(\mathbf{u}_{i+1})$$

Steger & Warming, van Leer, AUSM and variants

Roe scheme

exact solution to linear Riemann problem

$$\frac{\partial \mathbf{u}}{\partial t} + A_{LR}(\mathbf{u}_L, \mathbf{u}_R)\frac{\partial \mathbf{u}}{\partial \mathbf{x}} = 0$$



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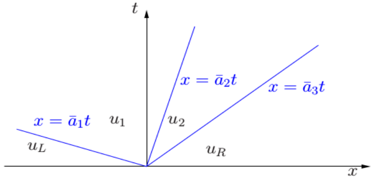

Properties of Roe matrix $\mathbf{A}_{LR}$

- $\mathbf{A}_{LR} \approx \mathbf{A}(\mathbf{u}) = D\mathbf{f}(\mathbf{u})$
- $\mathbf{A}_{LR}(\mathbf{u}, \mathbf{u}) = \mathbf{A}(\mathbf{u})$
- $\mathbf{A}_{LR}$ is diagonalizable
- $\mathbf{f}(\mathbf{u}_R) - \mathbf{f}(\mathbf{u}_L) = \mathbf{A}_{LR}(\mathbf{u}_R - \mathbf{u}_L)$ *(mean value property)*

entropy-fix needed

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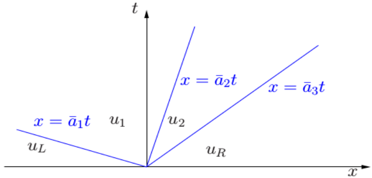
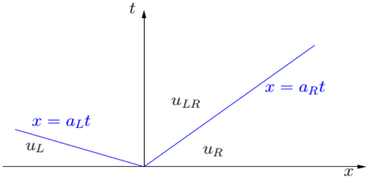


HLL scheme

Godunov-type scheme



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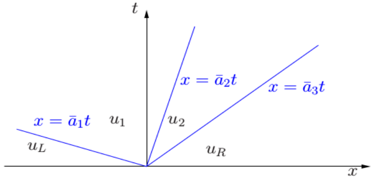

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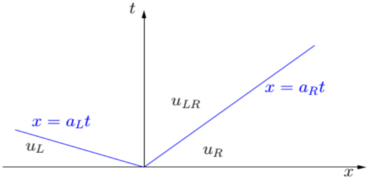
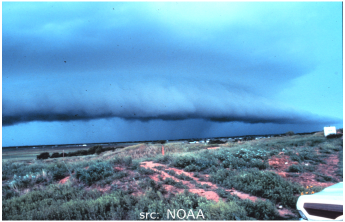


- approximates only one intermediate state
- based on integral conservation law

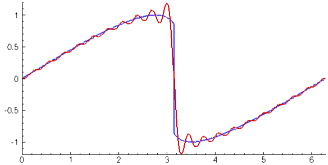
What about higher order schemes?

Challenges posed by hyperbolic conservation laws



gust front

bow waves



Oscillations of approximate solution

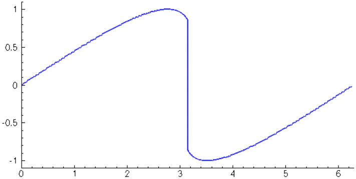
- Computation of discontinuous solutions (shocks)
- Unphysical oscillations
- Needs additional numerical dissipation

Difficulties regarding discontinuous solutions

Example: Burgers equation

$$\frac{\partial u}{\partial t} + u \cdot \frac{\partial u}{\partial x} = 0, \qquad u(x,0) = \sin(x)$$

Exact solution



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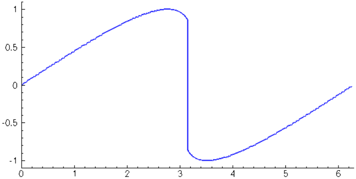
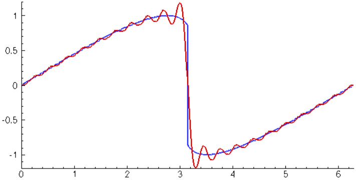


Projection



Goal: Controll oscillations

A first approach towards higher order

FV schemes with linear reconstruction – modify left and right states

$$u_i^{n+1} = u_i^n + \frac{\Delta x_i}{\Delta t}\left(f^*(u_i^n, u_{i+1}^n) - f^*(u_{i-1}^n, u_i^n)\right) = 0$$

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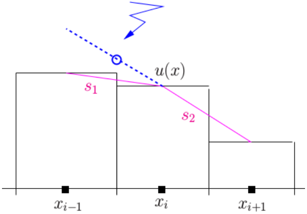

- linear reconstruction within cells $u(x) = u_i + s(x - x_i)$
- preserve integral means
- how to compute slopes s ?
- prevent creation of new max/min

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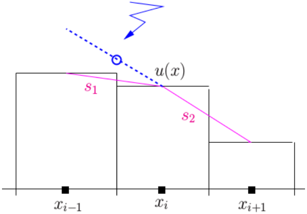


- linear reconstruction within cells $u(x) = u_i + s(x - x_i)$
- preserve integral means
- how to compute slopes s ?
- prevent creation of new max/min

enforce TVD property (relates to properties of exact solution)

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

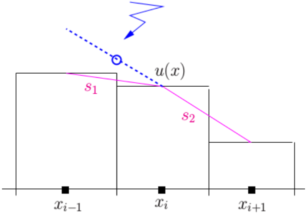
sufficient condition

$$0 \leq \left\{ \frac{\Delta x\, s_i}{u_i - u_{i-1}}, \frac{\Delta x\, s_i}{u_{i+1} - u_i} \right\} \leq 2$$

A first approach towards higher order

FV schemes with linear reconstruction – modify left and right states

$$u_i^{n+1} = u_i^n + \frac{\Delta x_i}{\Delta t}\left(f^*(u_i^n, u_{i+1}^n) - f^*(u_{i-1}^n, u_i^n)\right) = 0$$



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sufficient condition

$$0 \leq \left\{\frac{\Delta x\, s_i}{u_i - u_{i-1}}, \frac{\Delta x\, s_i}{u_{i+1} - u_i}\right\} \leq 2$$

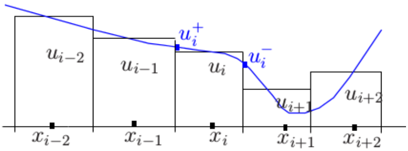
Typical example:

$s_i = \frac{1}{\Delta x}\text{minmod}(u_{i+1} - u_i, u_i - u_{i-1}),$

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

The ENO reconstruction

ENO stands for *essentially non-oscillatory*



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

The ENO reconstruction

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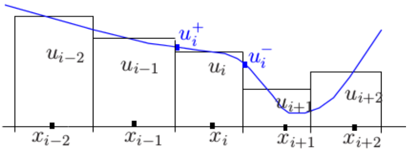

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ENO approach:

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

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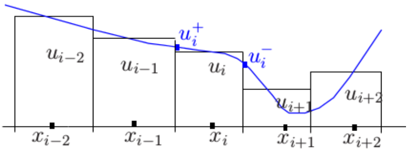


- higher order reconstruction via interpolation
- adaptively choose *stencil*
- avoid interpolation across shocks

ENO approach:

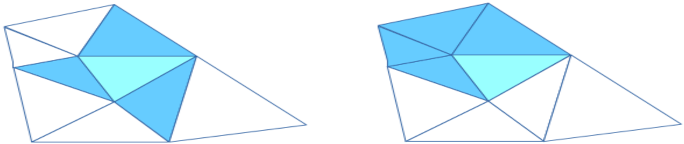
- successive increase of polynomial degree via Newton interpolation
- compare divided differences obtained by left or right extension

ENO properties:

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

The WENO reconstruction

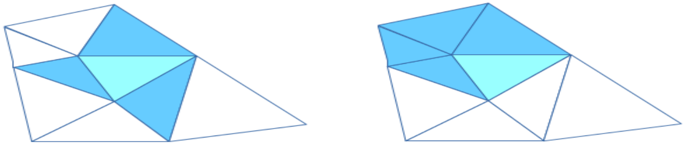
WENO stands for *weighted essentially non-oscillatory*



- 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

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

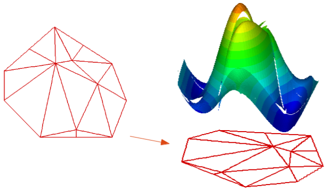
WENO properties:

- 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)

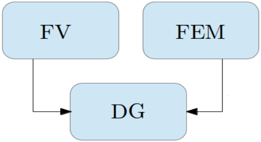
From Finite Volumes ...

.. to Discontinuous Galerkin

Discontinuous Galerkin schemes



discontinuous approximate solutions



modern space discretization

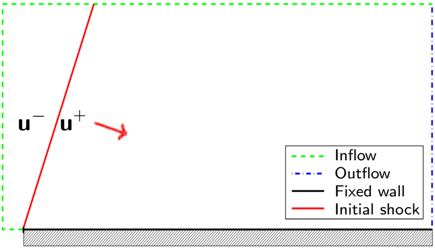
$$\frac{d}{dt}\int_{V_i} \mathbf{u}_h\,\Phi\,d\mathbf{x} + \int_{\partial V_i} \mathbf{F}^*(\mathbf{u}_h^-,\mathbf{u}_h^+,\mathbf{n})\,\Phi\,d\sigma - \int_{V_i} \mathbf{F}(\mathbf{u}_h)\cdot\nabla\Phi\,d\mathbf{x} = \int_{V_i} \mathbf{q}_h\,\Phi\,d\mathbf{x}$$

FV: $\Phi = \Phi_0$ $\leftrightarrow$ DG: $\Phi = \Phi_0, \Phi_1, \ldots, \Phi_N$

$\rightarrow$ Closer link to given physical equations

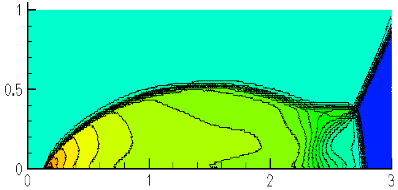
- High accuracy & flexibility
- Compact domains of dependance
- Highly adapted to computations in parallel

Double Mach reflection: Shock hitting fixed wall

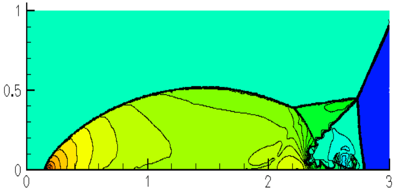


Excellent shock resolution
&
Detailed representation
of fine structures

Density distribution: FV vs. DG scheme



FV scheme



DG scheme ($N = 4$)

The triangular grid DG scheme

Hyperbolic conservation law in 2D

$$\frac{\partial}{\partial t}\mathbf{u}(\mathbf{x},t) + \nabla \cdot \mathbf{F}(\mathbf{u}(\mathbf{x},t)) = 0, \qquad (\mathbf{x},t) \in \Omega \times \mathbb{R}^+$$

Initial conditions:	$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x})$
Boundary conditions:	inflow/outflow, reflecting walls

The triangular grid DG scheme

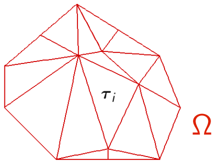
Hyperbolic conservation law in 2D

$$\frac{\partial}{\partial t}\mathbf{u}(\mathbf{x},t) + \nabla \cdot \mathbf{F}(\mathbf{u}(\mathbf{x},t)) = 0, \qquad (\mathbf{x},t) \in \Omega \times \mathbb{R}^+$$

Initial conditions: $\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x})$

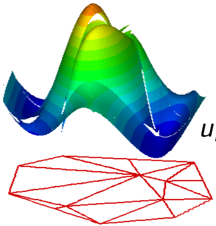
Boundary conditions: inflow/outflow, reflecting walls

Approximation $\mathbf{u}_{h,N}(\mathbf{x},t)$: piecewise polynomial in $\mathbf{x}$, degree $\leq N$



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

Triangulation



$u_{h,N}(\cdot, t)$

The triangular grid DG scheme

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

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

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Use divergence theorem

$$\frac{d}{dt}\int_{\tau_i} \underset{\substack{\uparrow\\ \mathbf{u}_{h,N}}}{\mathbf{u}}\,\Phi\, d\mathbf{x} + \int_{\partial\tau_i} \underset{\substack{\uparrow\\ \mathbf{F}^*(\mathbf{u}^-_{h,N},\,\mathbf{u}^+_{h,N},\,\mathbf{n})}}{\mathbf{F}(\mathbf{u})\cdot\mathbf{n}}\ \Phi\, d\sigma - \int_{\tau_i} \underset{\substack{\uparrow\\ \mathbf{F}(\mathbf{u}_{h,N})}}{\mathbf{F}(\mathbf{u})}\cdot\nabla\Phi\, d\mathbf{x} = 0$$

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$$\frac{d}{dt}\int_{\tau_i} \underset{\substack{\uparrow \\ \mathbf{u}_{h,N}}}{\mathbf{u}}\,\Phi\,d\mathbf{x} + \int_{\partial\tau_i} \underset{\substack{\uparrow \\ \mathbf{F}^*(\mathbf{u}_{h,N}^-,\,\mathbf{u}_{h,N}^+,\,\mathbf{n})}}{\mathbf{F}(\mathbf{u})\cdot\mathbf{n}}\;\Phi\,d\sigma - \int_{\tau_i} \underset{\substack{\uparrow \\ \mathbf{F}(\mathbf{u}_{h,N})}}{\mathbf{F}(\mathbf{u})} \cdot \nabla\Phi\,d\mathbf{x} = 0$$

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

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

With respect to orthogonal basis

Time Evolution of coefficients

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

Quadrature rules

With respect to orthogonal basis

Time Evolution of coefficients

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

Quadrature rules

$\rightarrow$ System of ODEs for coefficients $\hat{\mathbf{u}}_k^i$

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

With respect to orthogonal basis

Time Evolution of coefficients

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

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$\rightarrow$ e.g. Runge Kutta time integration

Cockburn and Shu (1989-91, 1998)

With respect to orthogonal basis

Time Evolution of coefficients

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

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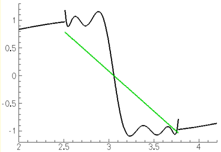
$\rightarrow$ e.g. Runge Kutta time integration

Cockburn and Shu (1989-91, 1998)

Allows easy incorporation of modal filters Meister, Ortleb, Sonar '12

Modify approximate solution

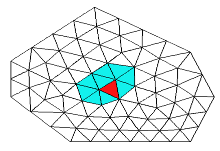
Limiters



– 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

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

– In conservation law or discretization
– Time step $\mathcal{O}(h^2)$

Jaffre,Johnson,Szepessy '95
Persson,Peraire '06
Feistauer,Kučera '07

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

Fourier method: $\frac{\partial}{\partial t}u_N + \frac{\partial}{\partial x}\mathcal{P}_N f(u_N) = 0$

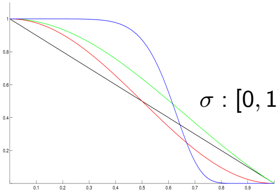
$$u_N(x,t) = \sum_{|k|\le N} \hat{u}_k(t) e^{ikx}$$

Modal Filtering

Modify coefficients at times t^n

$$u_N^\sigma(x,t^n) = \sum_{|k|\le N} \sigma\left(\frac{|k|}{N}\right) \hat{u}_k^n\, e^{ikx}$$

Gottlieb, Lustman, Orzag '81



$\sigma : [0,1] \to [0,1]$

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

$$\epsilon_N (-1)^{p+1} \frac{\partial^p}{\partial x^p}\left[Q_N \frac{\partial^p u_N}{\partial x^p}\right]$$

Tadmor '89

Damping for spectral methods

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Link $\longleftrightarrow$

Spectral viscosity

Add special viscosity term

$$\epsilon_N (-1)^{p+1} \frac{\partial^p}{\partial x^p}\left[Q_N \frac{\partial^p u_N}{\partial x^p}\right]$$

Simple implementation

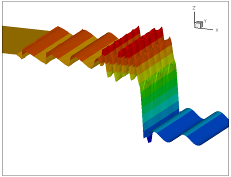
Convergence theory, Parameter choice

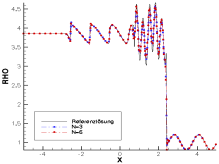
Initial conditions

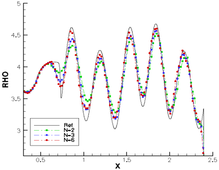
$$(\rho, v_1, v_2, p) = \begin{cases} (3.857143, 2.629369, 0, 10.333333) & \text{if } x < -4 \\ (1 + 0.2 \cdot \sin(5x), 0, 0, 1) & \text{if } x \geq -4 \end{cases}$$

DG with modal filtering

approximate density solution ($t = 1.8$)

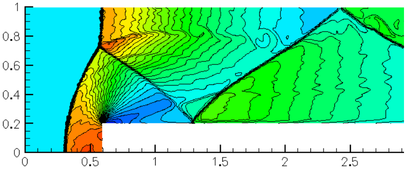






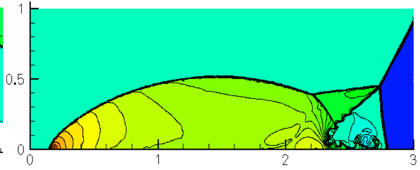
Discretization: $N = 5$, $K = 1250$

Further classical test cases



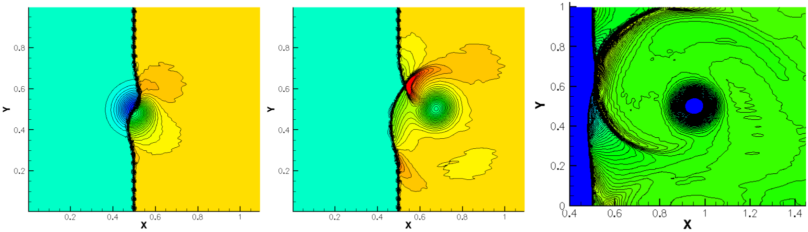
forward facing step

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

Conservative schemes in 1D

- Finite Volume Method
- Discontinuous Galerkin Method Cockburn/Shu '89
- Spectral Difference Method Kopriva/Kolias '96, Liu et al. '06, Wang et al. '07
- 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

Scalar hyperbolic conservation law in 1D

$$\frac{\partial}{\partial t}u(x,t)+\frac{\partial}{\partial x}f(u(x,t))=0, \quad t>0, x\in\Omega=[\alpha,\beta]$$

Subdivision of Ω in

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

approximation of u on Ω_i

$$u_h^i(x,t)=\sum_{k=1}^{N+1} u_l^i(t)\Phi_l^i(x) \qquad \text{with basis functions } \Phi_l^i$$

$$\underline{u}^i=(u_1^i,\dots,u_{p+1}^i)^T \qquad \text{solution vector}$$

The DG scheme in strong form

$$\int_{\Omega_i}\frac{\partial u_h^i}{\partial t}\Phi_k^i dx+\int_{\Omega_i}\frac{\partial f_h^i}{\partial x}\Phi_k^i dx=[f^*_{i-1,i}-f_h^i(x_i)]\Phi_k^i(x_i)-[f^*_{i,i+1}-f_h^i(x_{i+1})]\Phi_k^i(x_{i+1})$$

The 1D DG scheme

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$$\underline{u}^i = (u_1^i, \ldots, u_{p+1}^i)^T \qquad \text{solution vector}$$

The DG scheme in strong form

$$\int_{\Omega_i} \frac{\partial u_h^i}{\partial t}\Phi_k^i dx + \int_{\Omega_i} \frac{\partial f_h^i}{\partial x}\Phi_k^i dx = [f_{i-1,i}^* - f_h^i(x_i)]\Phi_k^i(x_i) - [f_{i,i+1}^* - f_h^i(x_{i+1})]\Phi_k^i(x_{i+1})$$

equivalent to

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

$$M_{kl}^i = \int_{\Omega_i} \Phi_k^i \Phi_l^i dx$$
$$S_{kl}^i = \int_{\Omega_i} \Phi_k^i \frac{\partial}{\partial x}\Phi_l^i dx$$
$$\underline{\Phi}^i = (\Phi_1^i, \ldots, \Phi_{p+1}^i)^T$$

SBP schemes

Generalized definition of 1D SBP scheme

Del Rey Fernández et al. '14

- $\underline{\underline{M}}$ symmetric positive definite
- $\underline{\underline{D}} := \underline{\underline{M}}^{-1}\underline{\underline{S}}$ approximates $\frac{\partial}{\partial x}$
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  SBP mimics **integration by parts**

Generalized definition of 1D SBP scheme

Del Rey Fernández et al. '14

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fulfilled by DG scheme

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

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

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

$$\underline{\underline{B}}_{GLL} = \text{diag}\{-1, 0, \dots, 0, 1\},$$

$$\underline{\underline{B}}_{GL,N=1} = \text{diag}\{-\sqrt{3}, \sqrt{3}\}, \quad \underline{\underline{B}}_{GL,N=2} = \begin{pmatrix} -\frac{1}{\xi^3} & \frac{1-\xi^2}{\xi^3} & 0 \\ \frac{1-\xi^2}{\xi^3} & 0 & \frac{\xi^2-1}{\xi^3} \\ 0 & \frac{\xi^2-1}{\xi^3} & \frac{1}{\xi^3} \end{pmatrix}, \quad \xi = \sqrt{\frac{3}{5}}$$

Advantages of SBP schemes

Provable linear stability

Energy stability w.r.t. $\frac{1}{2}\|\underline{\boldsymbol{u}}\|^2_{\underline{\underline{M}}}$

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Corresponding QF preserve certain properties of functional

e.g. discrete divergence theorem Hicken/Zingg '13

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

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- 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 $\leftrightarrow$ Energy Stable Flux Reconstruction (VCJH)

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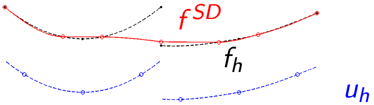
These methods meet as SBP schemes!

The SD scheme [Wang et al. '07]

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

Construction of f^{SD}



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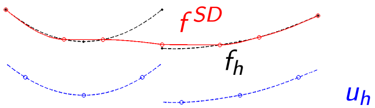

Generalized by FR scheme [Huynh '11]

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

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

DG for g_L, g_R right & left Radau polynomials

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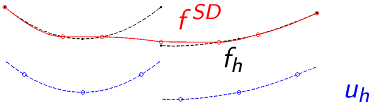

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in matrix-vector form [Allaneau/Jameson '11]

- expand u_h, f_h and g_L', g_R' in same basis $\{\Phi_k\}$
- multiply by $\underline{\underline{M}}$ with $M_{kl} = \int_{\Omega_i} \Phi_k \Phi_l dx$

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Spectral difference and flux reconstruction schemes

The SD scheme [Wang et al. '07]

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

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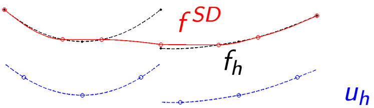

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Relation of FR framework to DG scheme

Reformulate

$$\underline{\underline{M}}\frac{d\underline{u}}{dt} + \underline{\underline{S}}\,\underline{f} = -f_{CL}\underline{\underline{M}}\,\underline{g}'_L - f_{CR}\underline{\underline{M}}\,\underline{g}'_R$$

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$$RHS_{FR} = \underbrace{f_{CL}\underline{\Phi}(x_i) - f_{CR}\underline{\Phi}(x_{i+1})}_{RHS_{DG}} + \underbrace{\int_{\Omega_i} (f_{CL}g_L + f_{CR}g_R)\,\underline{\Phi}'dx}_{\text{Deviation from DG}}$$

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⇒ Two equivalent formulations for FR scheme:

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$$\frac{d\underline{u}}{dt} + \underline{\underline{D}}\,\underline{f} = -f_{CL}\,\underline{g}'_L - f_{CR}\,\underline{g}'_R$$

VCJH schemes: energy stable FR

Derivation of energy stable FR schemes:

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- Choose g_L, g_R such that red terms vanish for suitable $\underline{\underline{K}}$

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  $\rightarrow$ "filtered DG scheme" [Allaneau/Jameson '11]

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  $\rightarrow$ "filtered DG scheme" [Allaneau/Jameson '11]
- Fulfills SBP property! $[\underline{\underline{D}} = \underline{\underline{M}}^{-1}\underline{\underline{S}} = (\underline{\underline{M}} + \underline{\underline{K}})^{-1}\underline{\underline{S}}]$

Comparison of low order DGSBP schemes

&

Use of kinetic energy preservation and skew-symmetric forms

Smooth solutions to 1D Navier-Stokes equations

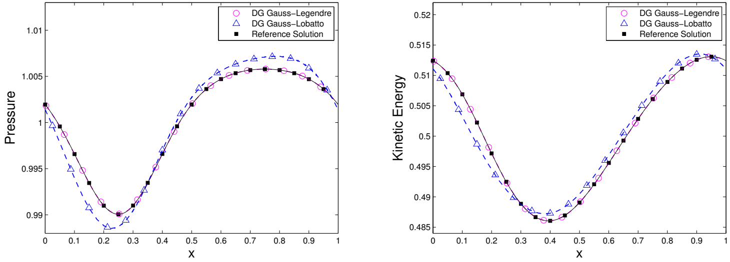
Non-linear acoustic pressure wave

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

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

Gauss-Legendre vs. Gauss-Lobatto nodes

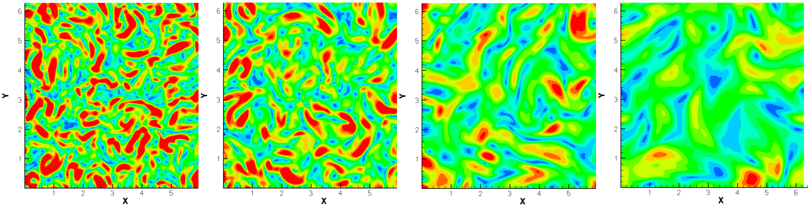
[$N = 1$ on 80 cells, KEP flux, $T = 20$; reference: $N = 3$ on 500 cells]



Higher accuracy of Gauss-Legendre DG scheme.

2D decaying homogeneous turbulence

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



$T = 1$ $T = 2$ $T = 5$ $T = 10$

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

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

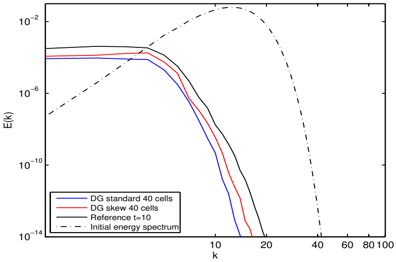
for wave number $k = \sqrt{k_x^2 + k_y^2}$ (Parameters $k_p = 12, a_s = \frac{7^4}{48}$)

Comparison standard DG vs. DG-KEP scheme (I)

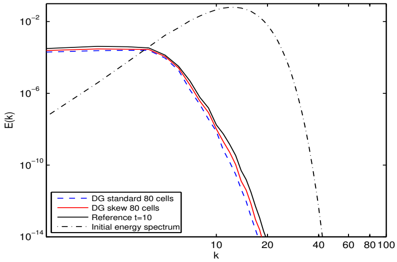
Energy spectrum $T = 10$

Gauss nodes, $N = 1$

Re=100



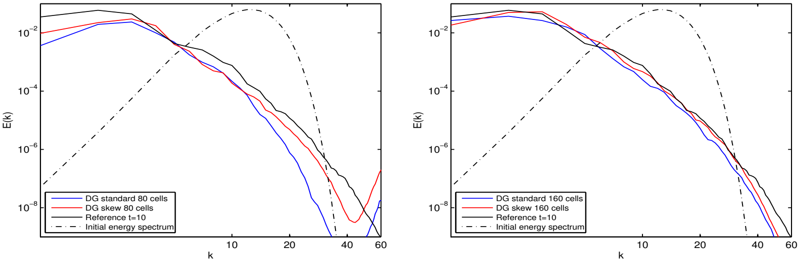
40×40 cells



80×80 cells

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

Re=600



80 × 80 cells

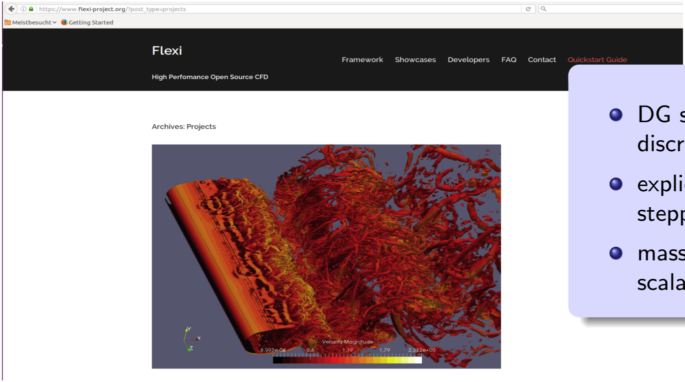
160 × 160 cells

Better representation of energy spectrum for KEP scheme.
Specifically for in underresolved case.

Current successful implementations

of DG and FR schemes

https://www.flexi-project.org

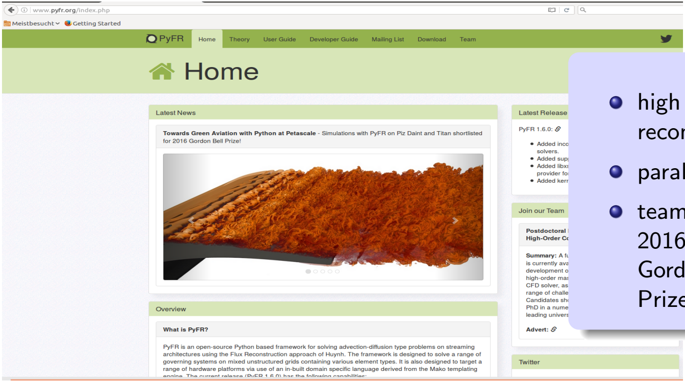


- DG space discretization
- explicit time stepping
- massive scalability

F. Hindenlang, G. J. Gassner, C. Altmann, A. Beck, M. Staudenmaier, C. Munz, "Explicit discontinuous Galerkin methods for unsteady problems", Computers & fluids 61, pp. 86–93, 2012.

Flux reconstrution with Python: PyFR

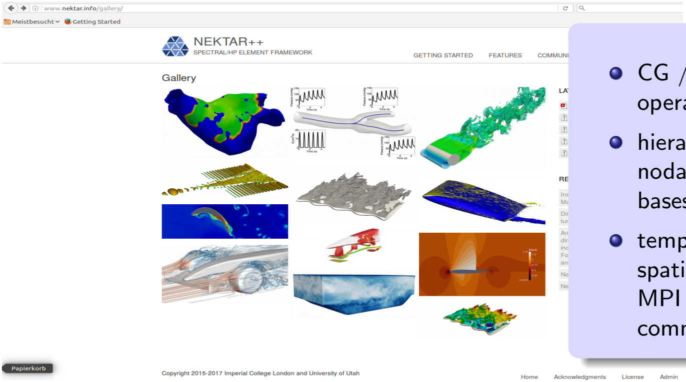
http://www.pyfr.org/index.php



- high order flux reconstruction
- parallel platforms
- team named a 2016 finalist for Gordon Bell Prize

F. D. Witherden, A. M. Farrington, P. E. Vincent, "PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach", Computer Physics Communications 185, pp. 3028–3040, 2014.

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



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

C. D. Cantwell, D. Moxey, A. Comerford, A. Bolis, G. Rocco, G. Mengaldo, D. De Grazia, S. Yakovlev, J.-E. Lombard, D. Ekelschot, B. Jordi, H. Xu, Y. Mohamied, C. Eskilsson, B. Nelson, P. Vos, C. Biotto, R.M. Kirby, S.J. Sherwin, "Nektar++: An open-source spectral/ element framework", Computer Physics Communications 192, pp. 205–219, 2015.

DG for OpenFOAM ?

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

- developement 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

N. Müller, S. Krämer-Eis, F. Kummer, M. Oberlack, "A high-order discontinuous Galerkin method for compressible flows with immersed boundaries", Int. J. Numer. Meth. Engng. 110, pp. 3–30, 2017.

Summary

Thank you for your attention!