On High-Order Space-Time Methods for CFD

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Motivation

- Effective spatial discretization is provided by Discontinuous Galerkin (DG) or Flux Reconstruction (FR) methods.

- Time discretization with such spatial methods results in

  1) either a small time step size in the case of an explicit time stepping, e.g., Runge-Kutta (Cockburn and Shu 1989,…)

  2) or a large system of equations in the case of an implicit time stepping such as space-time DG (Johnson and Pitkäranta 1986, Hughes and Hulbert 1988, Bar-Yoseph and Elata 1990, Van der Vegt and Van der Ven 2001, …)

- Efforts to improve time stepping has had limited success (staggered-mesh scheme, Warburton and Hagstrom 2008; singly diagonal implicit RK scheme, Vermeire et al. 2013, …)

- Time stepping is one of the pacing items mentioned by the committee of the International Workshop on High-order CFD methods (2011, 2013, 2014, 2016).
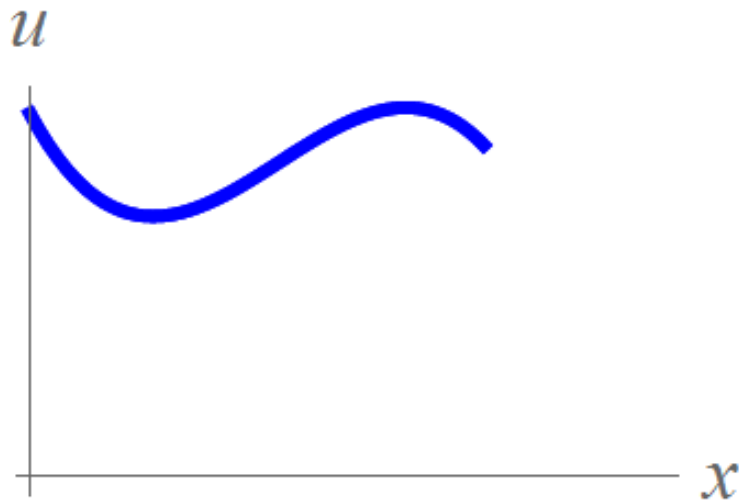
Outline

- Review of first-order (piecewise constant) methods

- Extensions to arbitrary order

  o Finite volume: Van Leer's MUSCL approach (piecewise linear case, scheme III, 1977), explicit method

  o Space-time finite element method: Johnson and J. Pitkäranta 1986, "An analysis of the discontinuous Galerkin method for a scalar hyperbolic equation", explicit and implicit methods

- Current efforts in extending to systems of equations and multi-dimensions

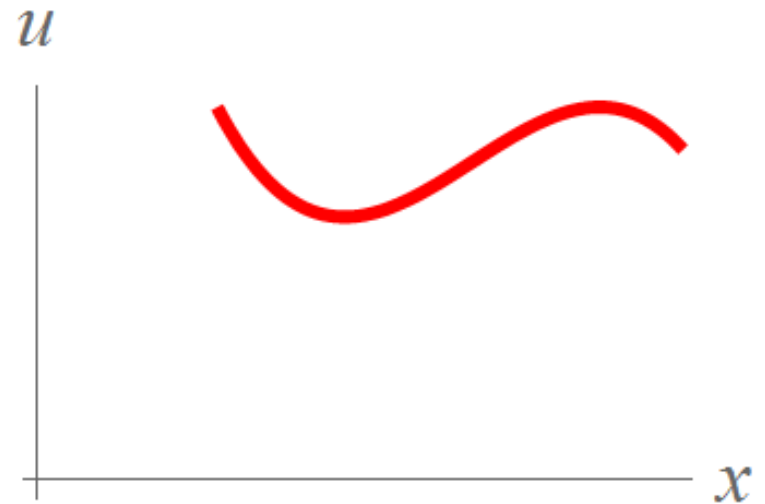- Conclusions

Advection Equation

$$u_t + au_x = 0, \quad a \geq 0$$

Initial condition : at $t = 0$, $u(x) = u_0(x)$
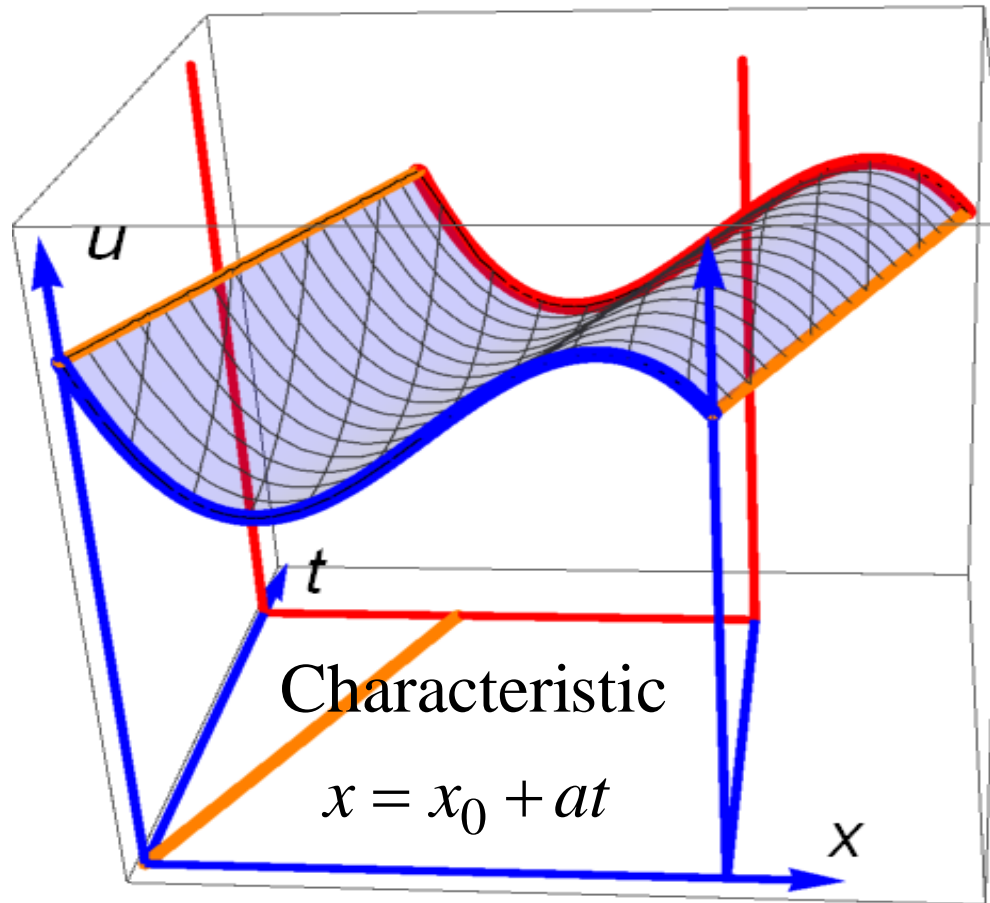
Exact solution : $u(x,t) = u_0(x - at)$

time $t = 0$

time $t > 0$

Exact Solution for Advection Equation
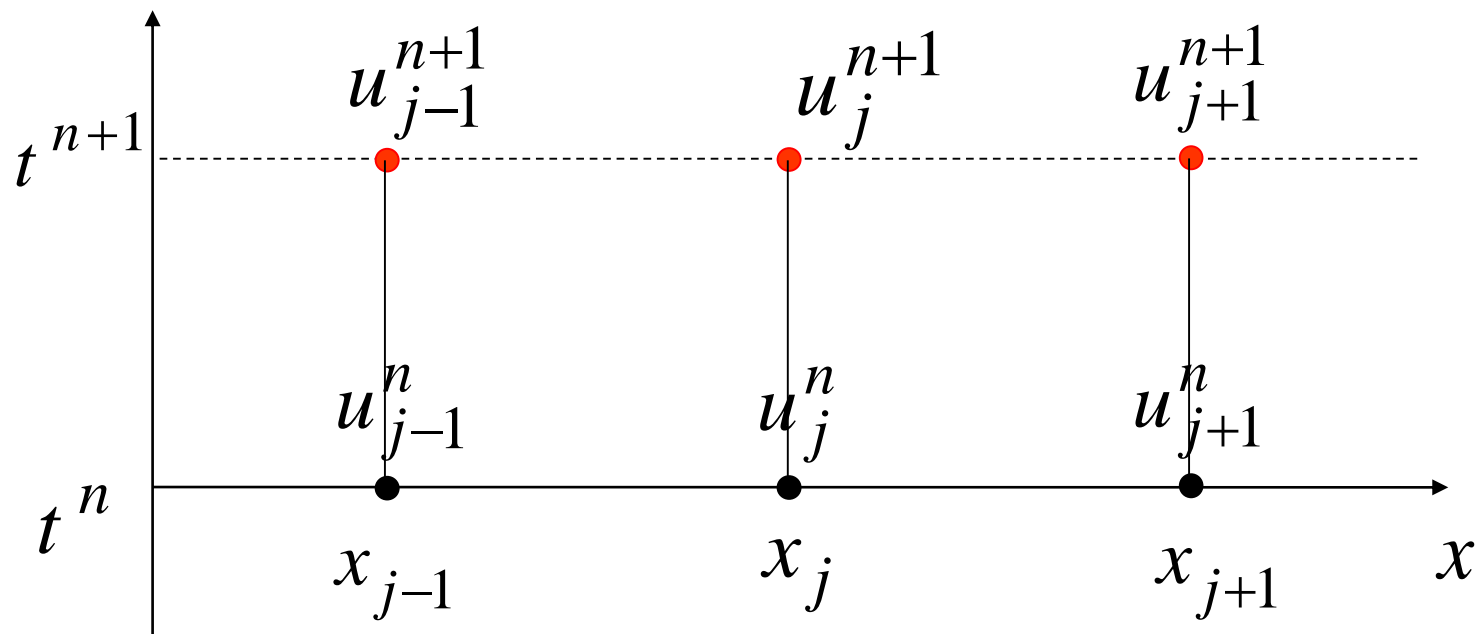

Characteristic

$$x = x_0 + at$$

Advection Equation

$$u_t + au_x = 0, \quad a \geq 0$$

The data at time t^n are known.

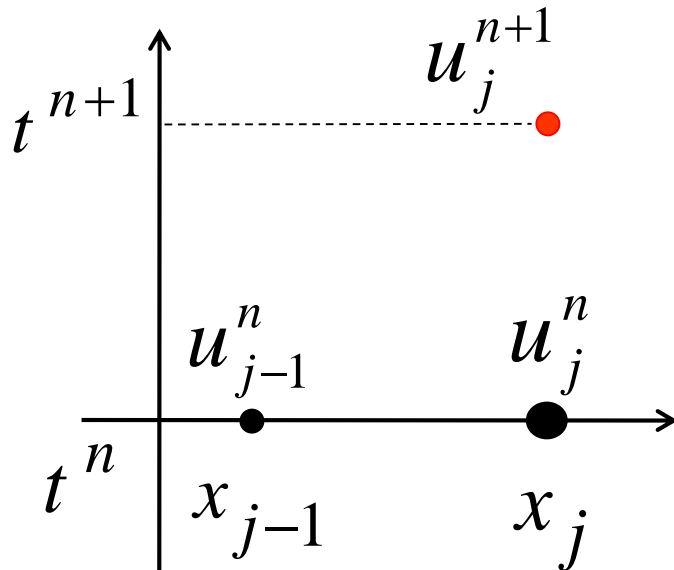Wish to calculate the solutions at time t^{n+1}

First-Order Upwind Explicit Method

$$u_t + a\,u_x = 0, \quad a \geq 0$$

Finite difference : Discretize at (j, n) using backward difference in space and forward difference in time

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\,\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0$$
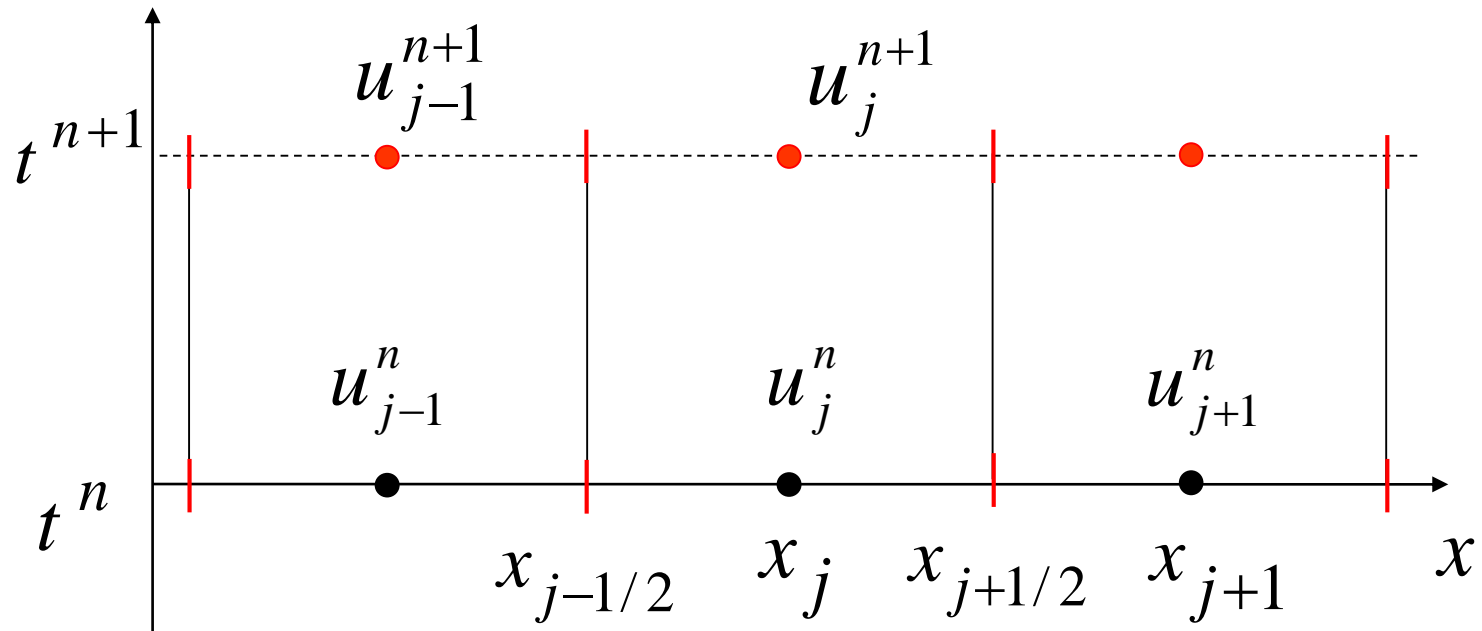
$$u_j^{n+1} = u_j^n - \left(a\,\frac{\Delta t}{\Delta x}\right)\left(u_j^n - u_{j-1}^n\right)$$

Or

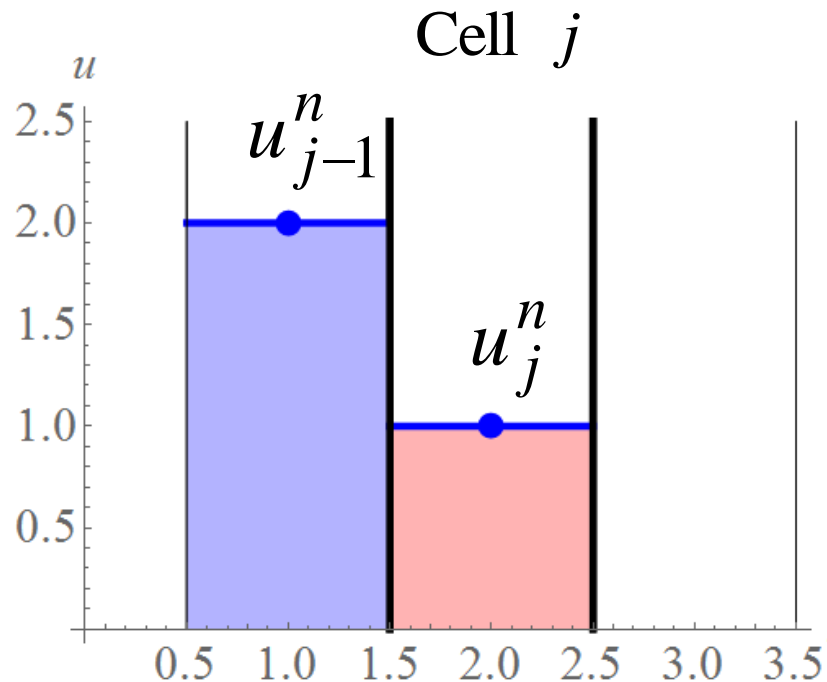$$u_j^{n+1} = u_j^n - \sigma\left(u_j^n - u_{j-1}^n\right)$$

Finite Volume Approach

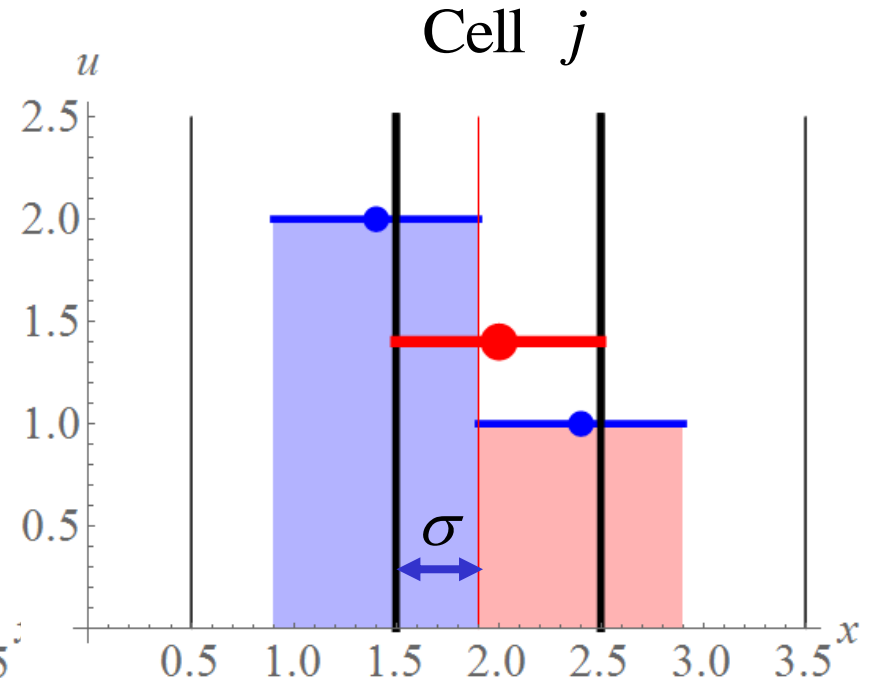The data u_j^n represents the average value of u in the cell $[x_{j-1/2}, x_{j+1/2}]$ at time t^n

First-order upwind method for advection: shift operator and projection
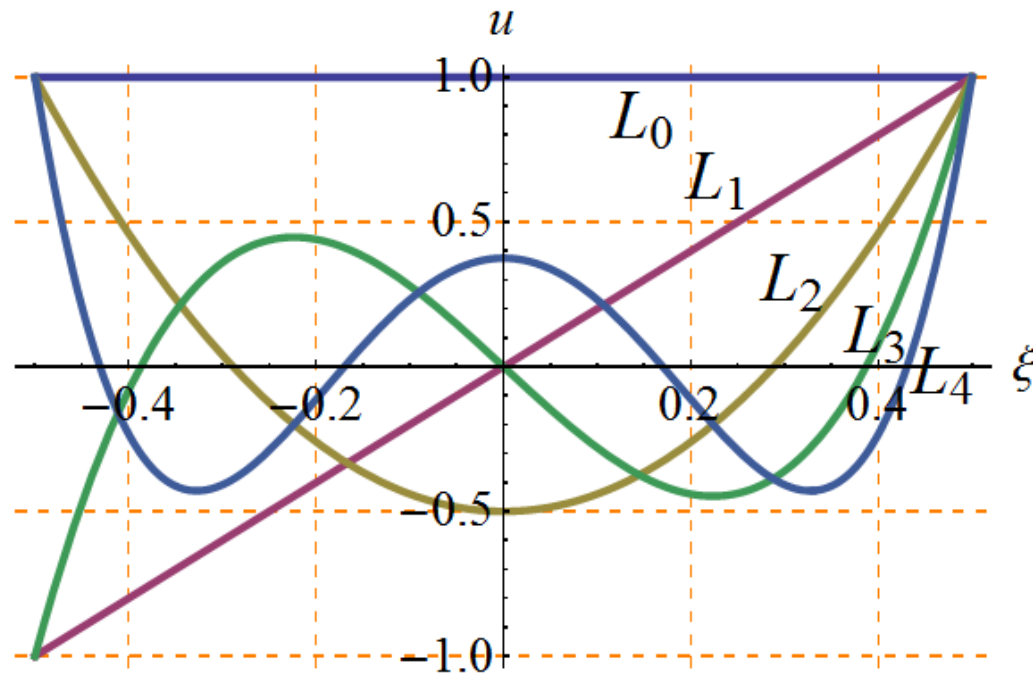
Cell j

Cell j

u_{j-1}^n

u_j^n

σ

(a) Data

(b) First-order solution (red)

$$u_j^{n+1} = u_j^n - \sigma\left(u_j^n - u_{j-1}^n\right)$$
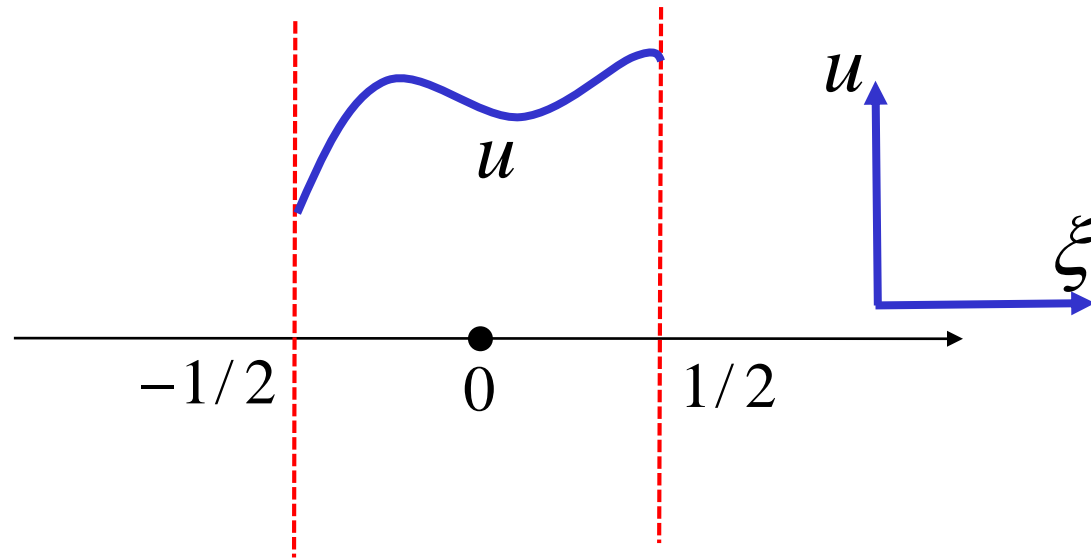
$$= \sigma u_{j-1}^n - (1-\sigma)u_j^n$$

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High-Order Extension Using Legendre Polynomials

By orthgonalizing the basis ξ^k, $k = 0, 1, 2, ...,$ via Gram - Schmidt process, we obtain the Legendre polynomials

$$L_0 = 1, \ L_1 = 2\xi, \ L_2 = 6\xi^2 - 1/2, ...$$

Projection using Legendre Polynomials

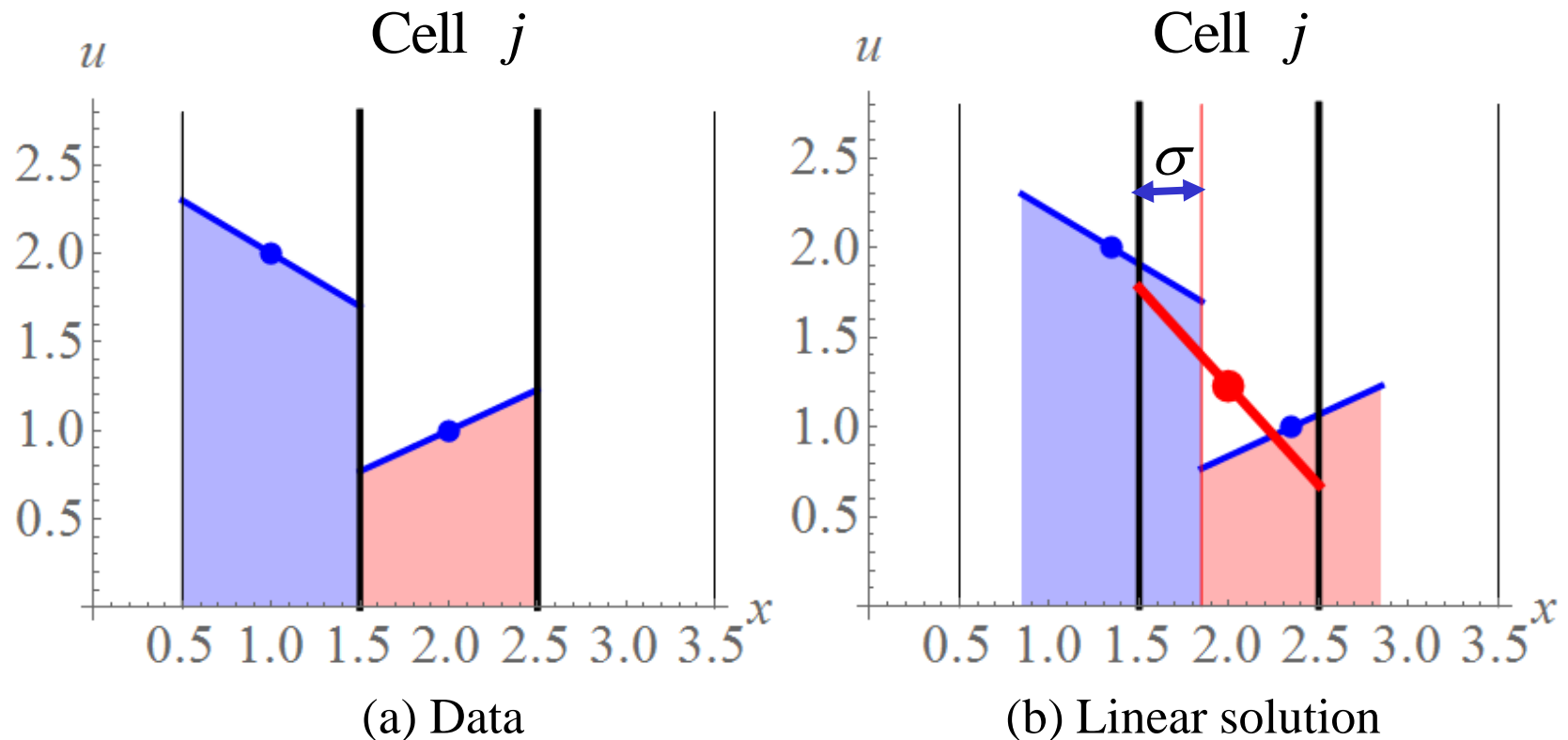On $I = [-1/2,\ 1/2]$, approximate u by $\sum_{k=0}^{p} u_{j,k}\, L_k$ where

$$u_{j,\,0}\ =\ \int_{-1/2}^{1/2} 1\, u(\xi)\, d\xi\,,$$

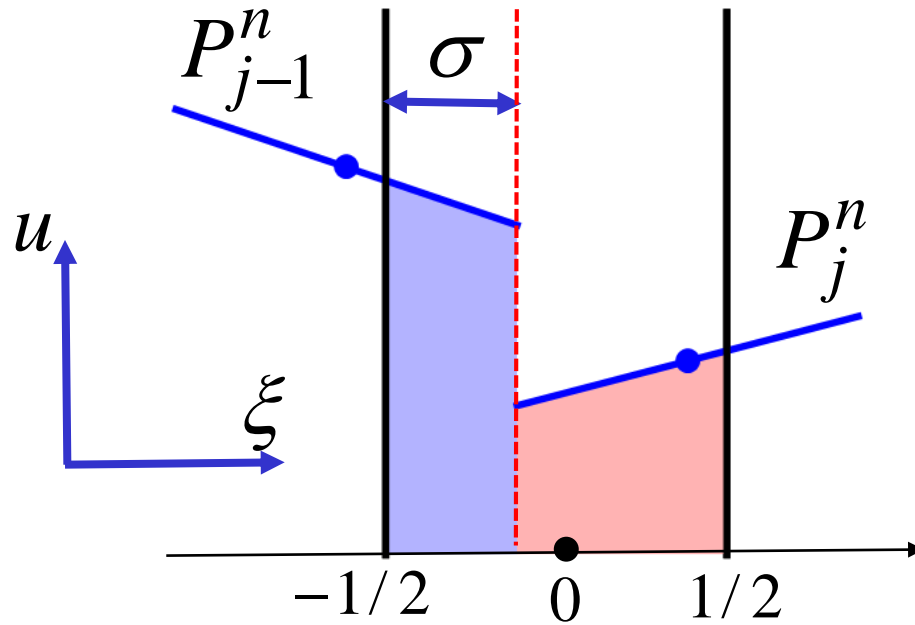$$u_{j,\,1}\ =\ \int_{-1/2}^{1/2} L_1(\xi)\, u(\xi)\, d\xi \Big/ \|L_1\|^2\,,$$

$$...$$

$$u_{j,\,k}\ =\ \int_{-1/2}^{1/2} L_k(\xi)\, u(\xi)\, d\xi \Big/ \|L_k\|^2$$
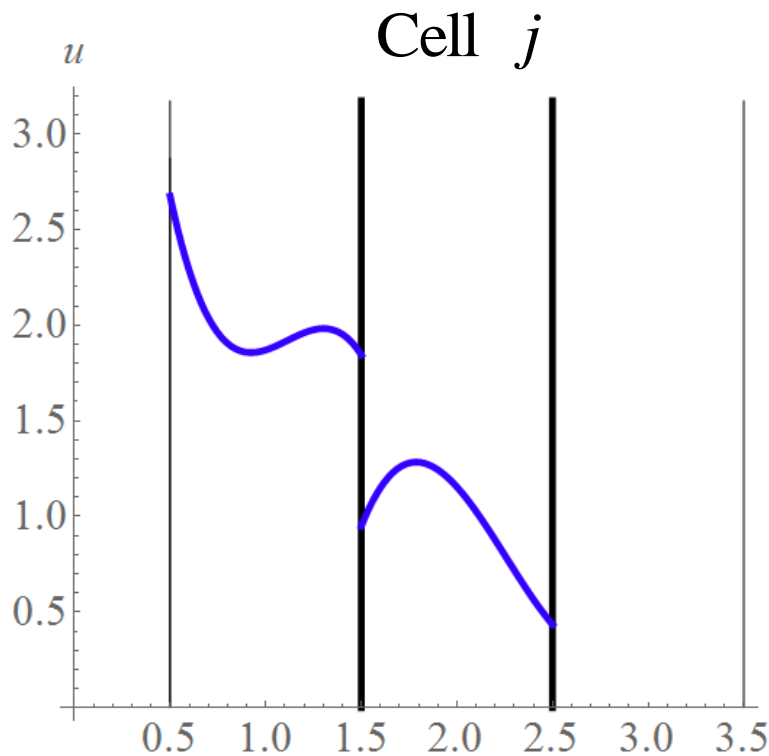
Van Leer's Scheme III Employing Shift and Projection

(a) Data

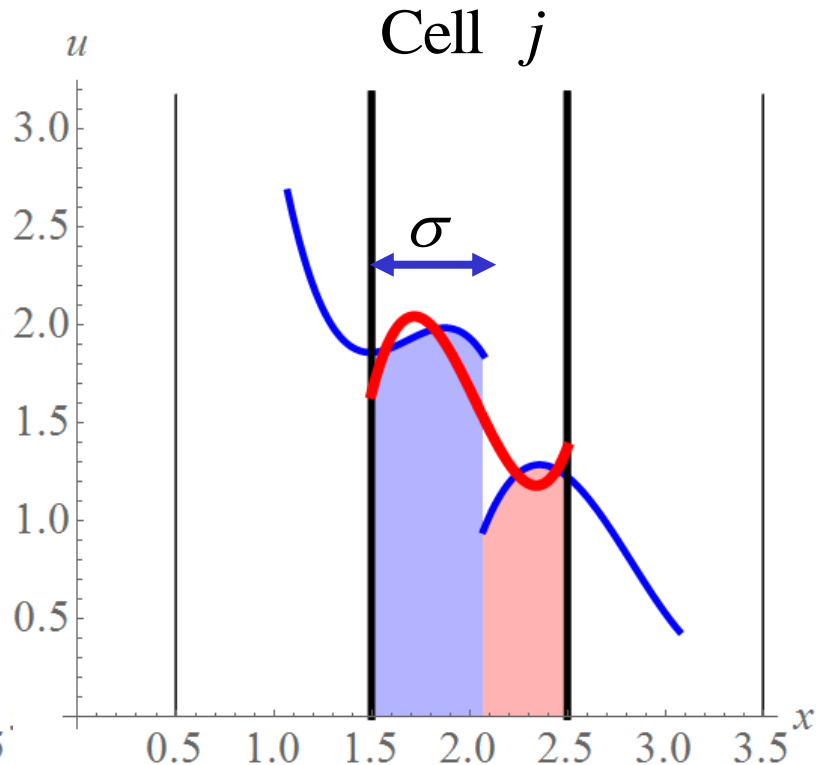(b) Linear solution

Van Leer's Scheme III (1977)

$$u_{j,\,k}^{n+1} = \left(\begin{array}{c} \displaystyle\int_{-1/2}^{-1/2+\sigma} P_{j-1}^{n}(\xi - \sigma + 1)\, L_k(\xi)\, d\xi \\[2mm] + \displaystyle\int_{-1/2+\sigma}^{1/2} P_{j}^{n}(\xi - \sigma)\, L_k(\xi)\, d\xi \end{array} \right) \Bigg/ \; \|L_k\|^2$$

$$P_j^{n+1}(\xi) = \sum_{k=0}^{p} u_{j,\,k}^{n+1}\, L_k(\xi)$$

Extension to Arbitrary Order (Below, Cubic) Employing Shift and Projection

(a) Data

(b) Solution (red curve)

Fourier Stability and Accuracy Analysis

$$u_t + au_x = 0, \quad a \geq 0$$

Initial condition : $u_0(x) = e^{iwx}$

Exact solution : $u(x,t) = e^{iw(x-at)} = e^{-iwat} e^{iwx}$

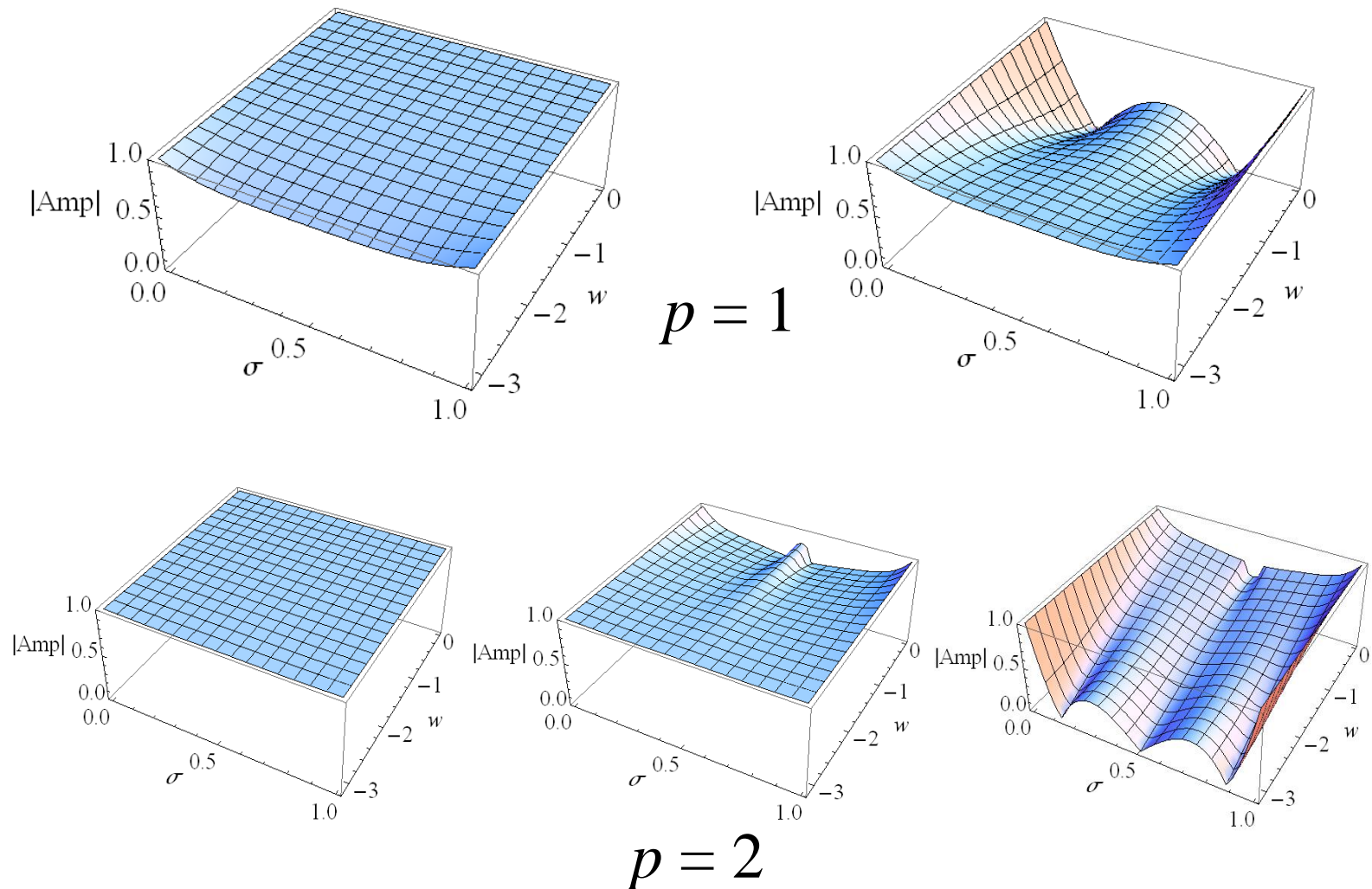To analyze numerical methods, assume $\Delta x = 1,\ x_j = j,$

$$u_0(x_j) = e^{iwx_j}$$

For time step $\Delta t,$ with $\sigma = a\Delta t / \Delta x,$ the exact solution is

$$u(x_j, \Delta t) = e^{-iw\sigma} e^{iwx_j}$$

A numerical method approximates $e^{-iw\sigma}$ by its
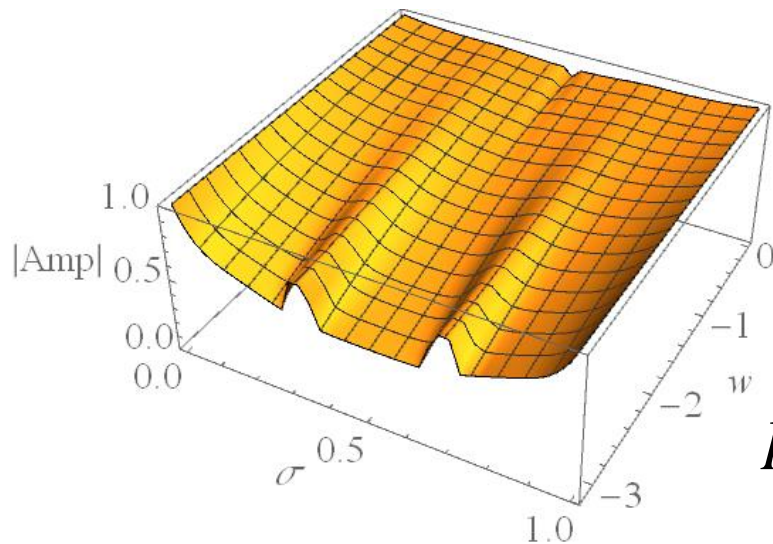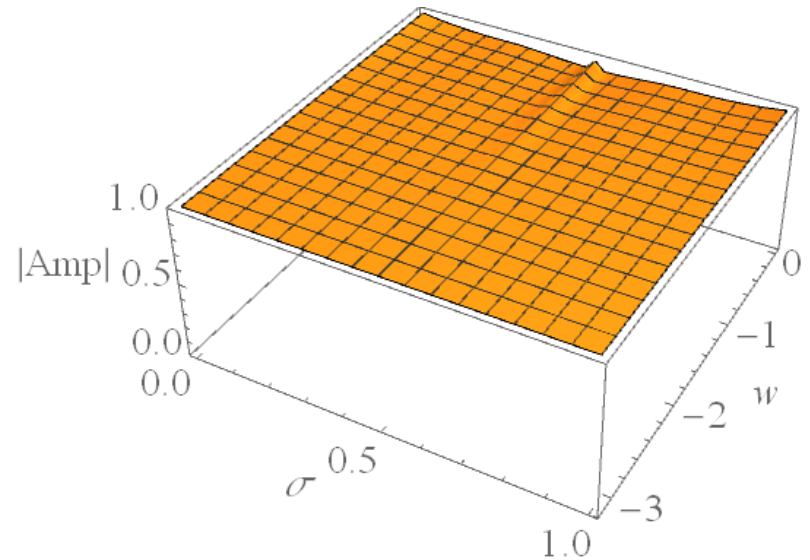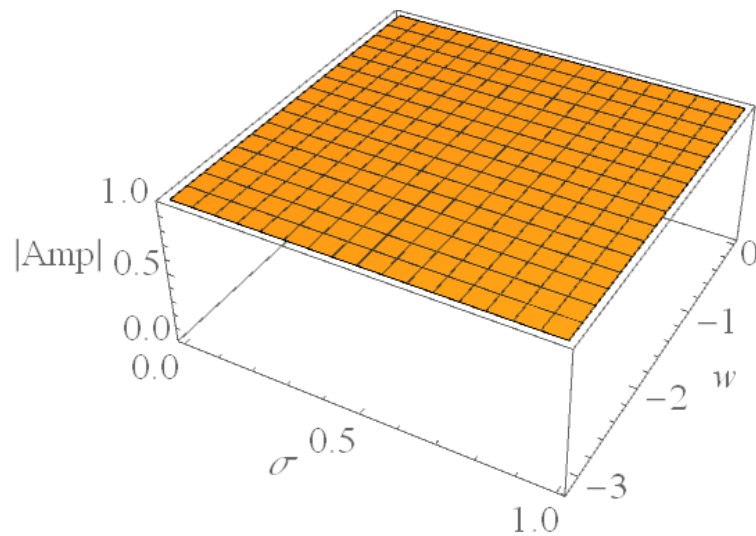
amplification factors (eigenvalues). Note that

$$\left| e^{-iw\sigma} \right| = 1.$$

Fourier Analysis: Plots of Absolute Values of Eigenvalues
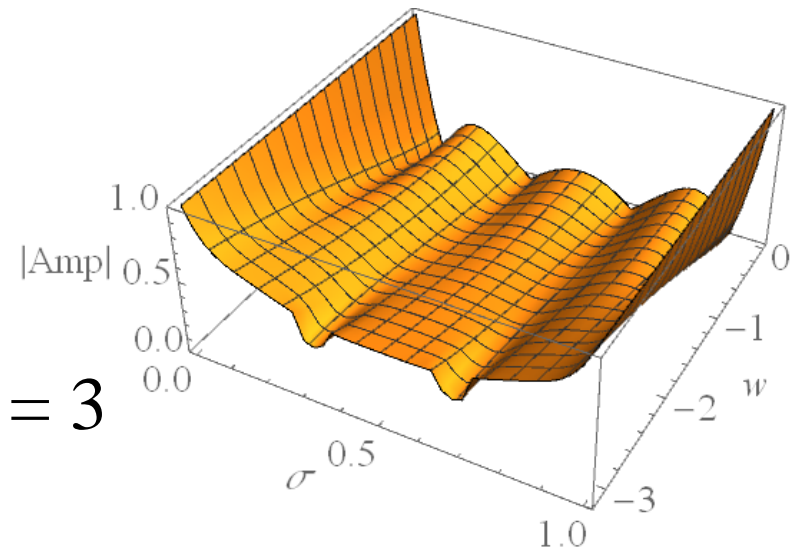

$$p = 1$$

$$p = 2$$

Fourier Analysis: Plots of Absolute Values of Eigenvalues

$p = 3$

Van Leer's scheme 3 (1977)

- Derived for advection equation

- <u>Uses projection</u> via Legendre polynomials (similar to DG)

- Piecewise linear method ($p = 1$) is third-order accurate; piecewise parabolic ($p = 2$), fifth-order. Degree p method is accurate to order $2p + 1$

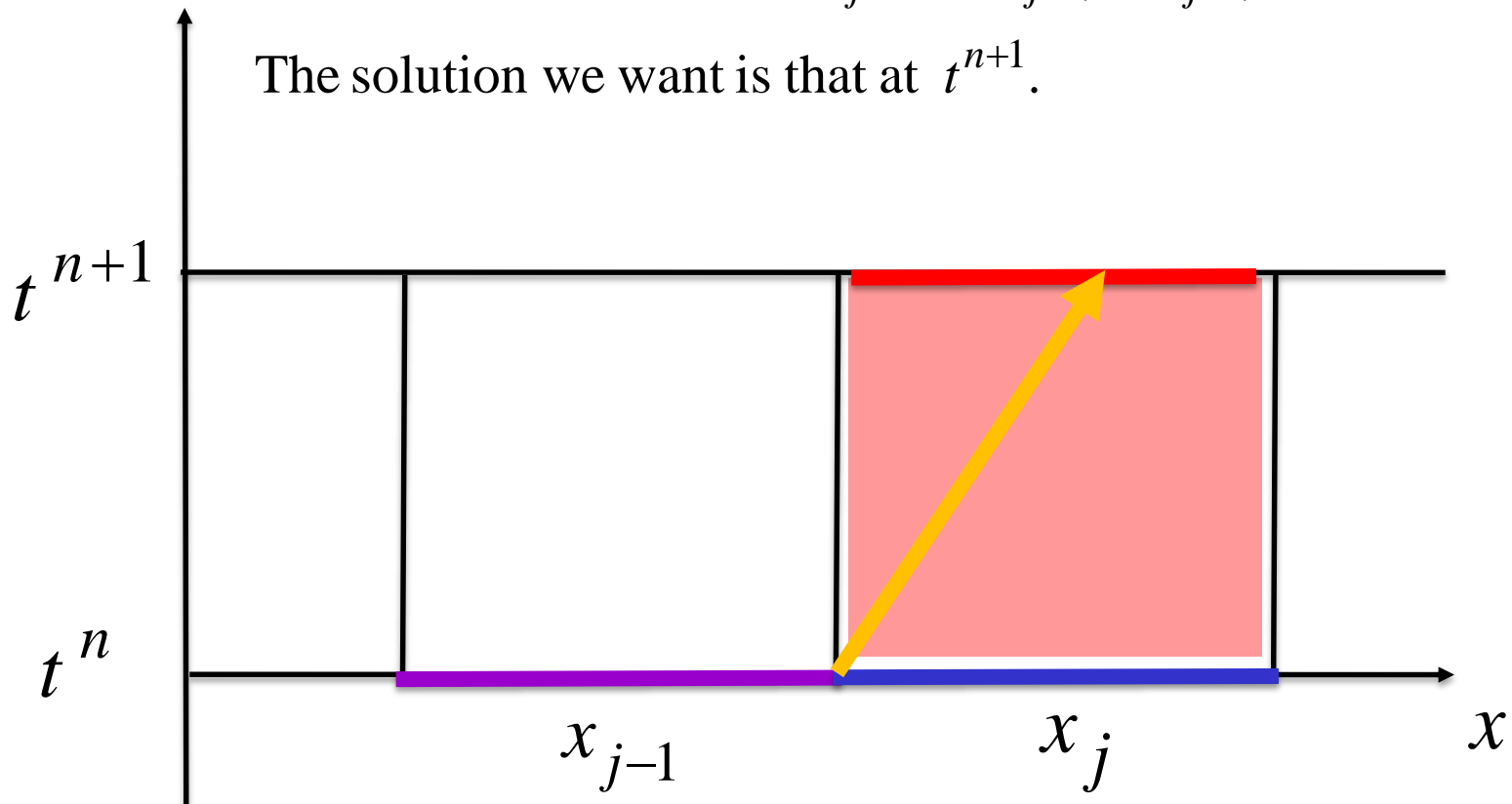- CFL condition is 1 as opposed to $\sim 1/(p + 1)^2$ for explicit RK-DG.

Difficulty

Concerning the extension of scheme III, Van Leer wrote (AIAA, Van Leer and Nomura 2005):

"When trying to extend these schemes beyond advection, viz., to a nonlinear hyperbolic system like the Euler equations, the first author ran into *insuperable* difficulties because the exact shift operator no longer applies, ..."
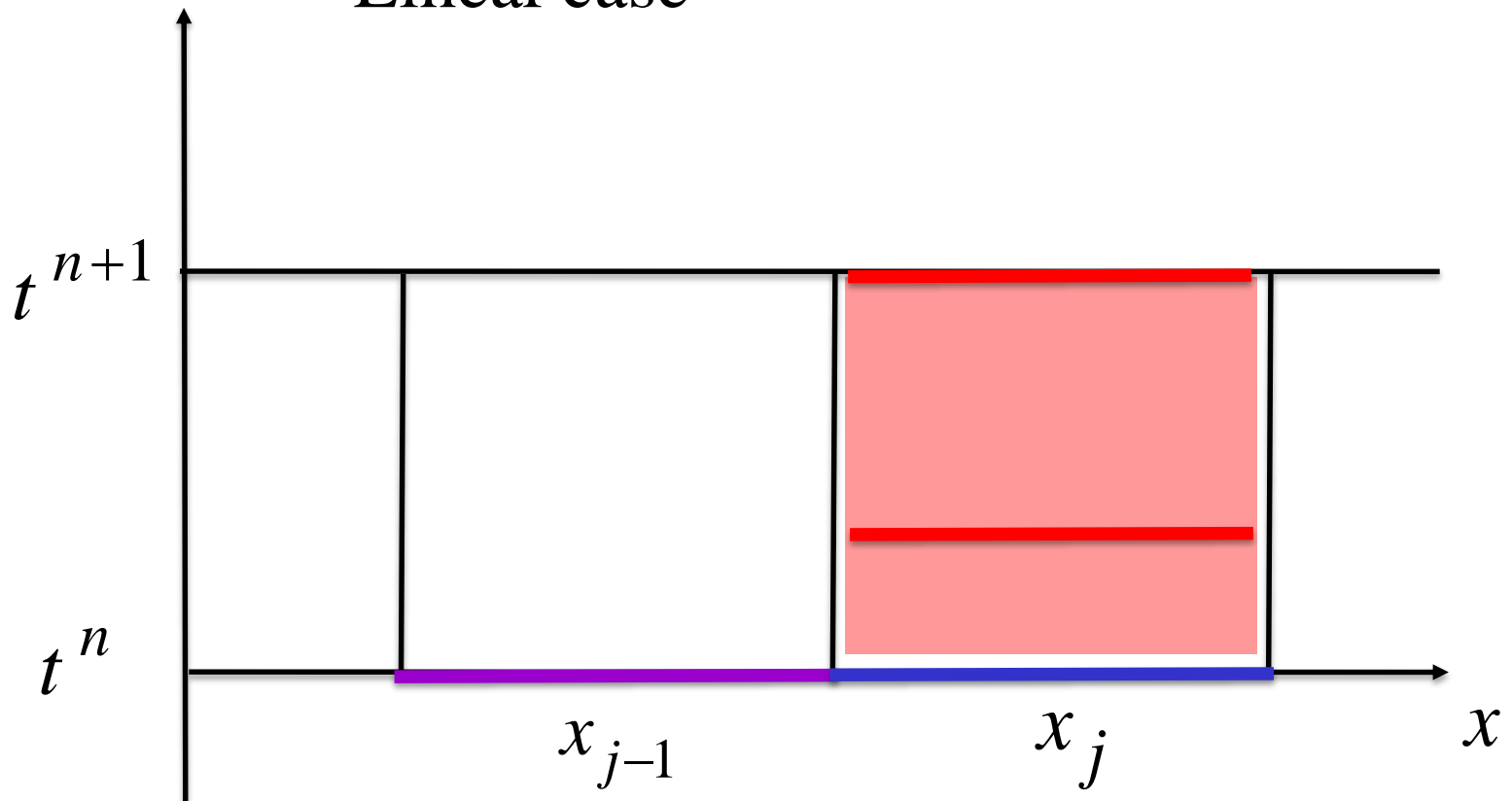
Extension to Systems via Space-Time Method

The data at time t^n are known for all spatial cells (polynomials of degree k). Wish to calculate the solution on each space-time cell $K_j^{n+1} = [x_{j-1/2}, x_{j+1/2}] \times [t^n, t^{n+1}]$. The solution we want is that at t^{n+1}.
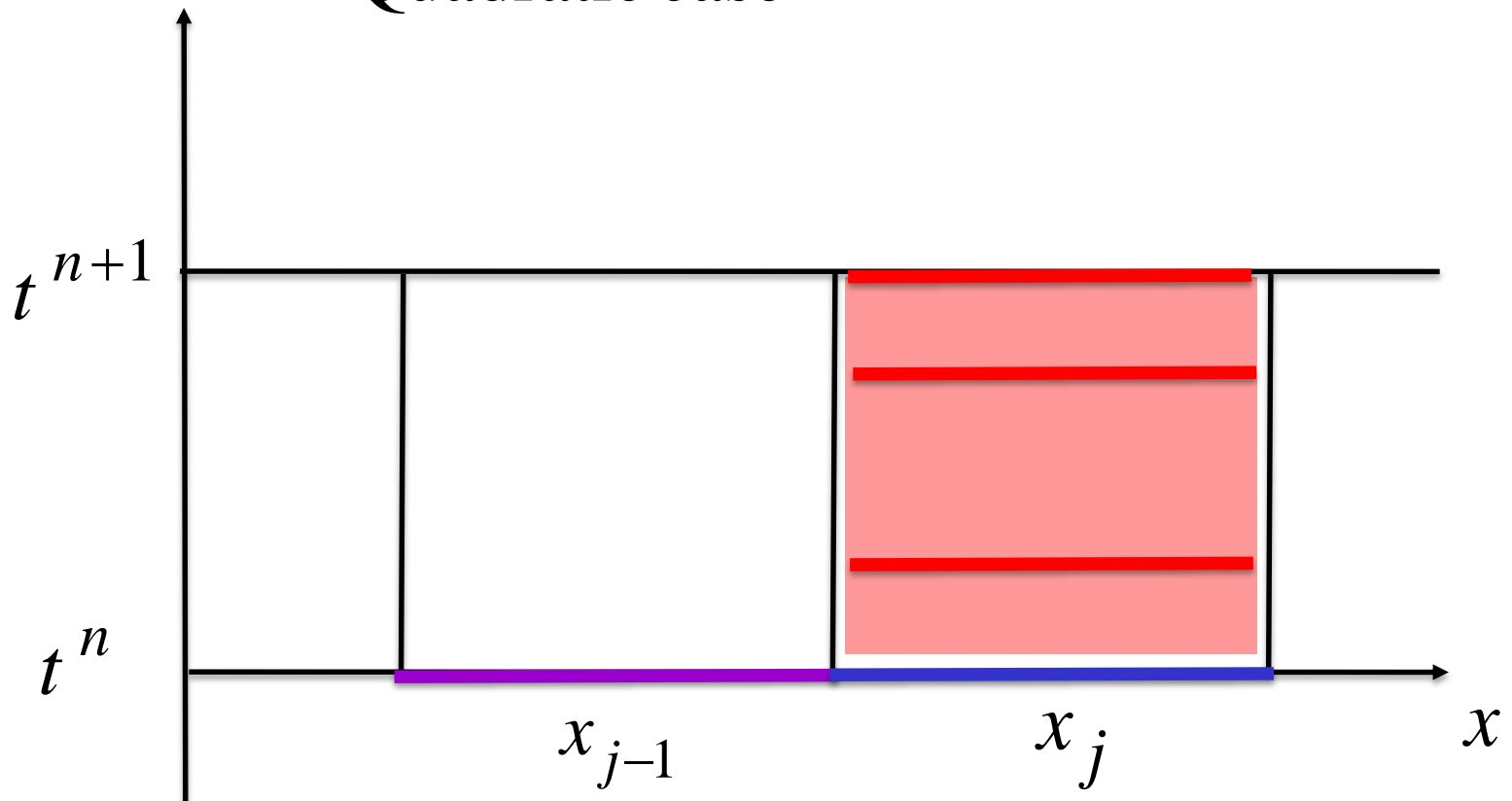
Space-Time Method

Right Radau quadrature points in time.

Linear case

Space-Time Method

Right Radau quadrature points in time.

Quadratic case

Moment Scheme

Solve $\qquad\qquad\qquad u_t + f_x = 0.$

On spatial cell E, require $\quad \int_E (u_t + f_x)\, \phi \; dx \; = \; 0.$

Integrate by parts

$$\frac{\partial}{\partial t} \int_E u\, \phi\; dx \; + \; \left[f_{\text{upw}}\phi \right]_{x_{j-1/2}}^{x_{j+1/2}} \; - \; \int_E f\, \phi_x\, dx \; = \; 0.$$

Here, $f_{\text{upw}}(x_{j-1/2})$ and $f_{\text{upw}}(x_{j+1/2})$ are **upwind** fluxes.

Integrate in time from t^n to t^*

$$\int_E u(x,t^*)\, \phi(x)\, dx - \int_E u(x,t^n)\, \phi(x)\, dx$$

$$+ \int_{t^n}^{t^*} \left[f_{\text{upw}}\phi \right]_{x_{j-1/2}}^{x_{j+1/2}} dt - \int_{t^n}^{t^*} \int_E f\, \phi_x\, dx\, dt \; = \; 0.$$

Moment Scheme

$$\int_E u(x, t^*) \, \phi(x) \, dx \;=\; \int_E u(x, t^n) \, \phi(x) \, dx$$

$$-\int_{t^n}^{t^*} \left[f_{\text{upw}} \phi \right]_{x_{j-1/2}}^{x_{j+1/2}} dt \;+\; \int_{t^n}^{t^*} \int_E f \, \phi_x \, dx \, dt$$

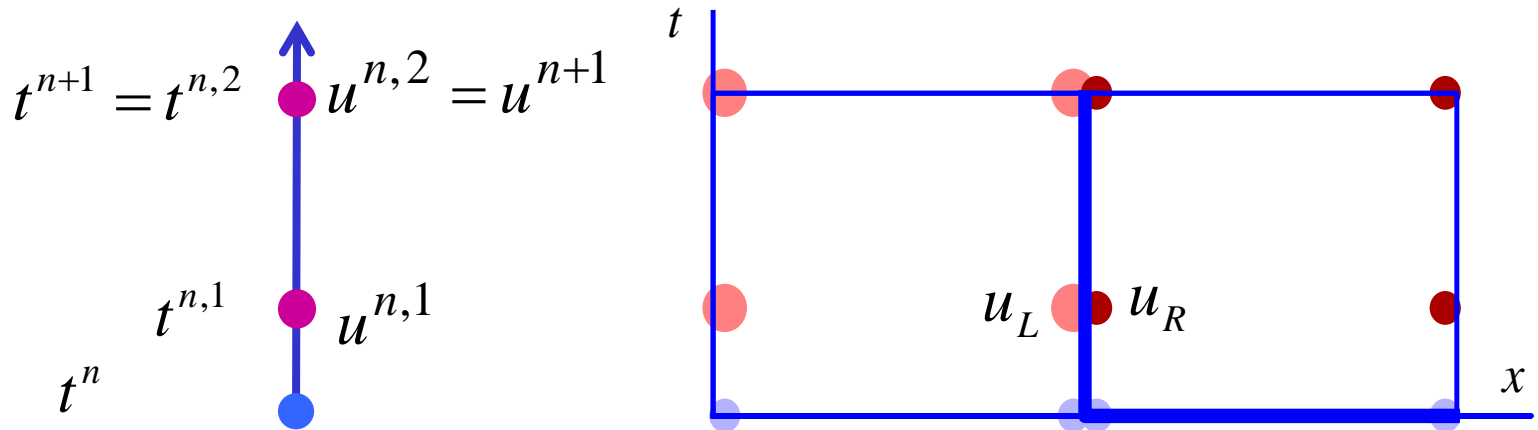$$\uparrow \qquad\qquad\qquad \uparrow$$

Surface Integral   Volume Integral

Moment Scheme
Time integration using right Radau points

Denote the data at purple dots by $u^{n,1}_{j,k}$ $(\tau = 1/3)$ and $u^{n,2}_{j,k}$ $(\tau = 1)$

We need quadratures for time integral from t^n to $t^{n,k}$

i.e., with τ on $[0,1]$, integral from 0 to c_k is given by,

$$\int_0^{1/3} u(\tau)\,d\tau = \frac{5}{12}u^{n,1} - \frac{1}{12}u^{n,2}$$

$$\int_0^1 u(\tau)\,d\tau = \frac{3}{4}u^{n,1} + \frac{1}{4}u^{n,2}$$

Cauchy-Kowalewsky Procedure for Polynomial Data (No Interaction Among Cells)
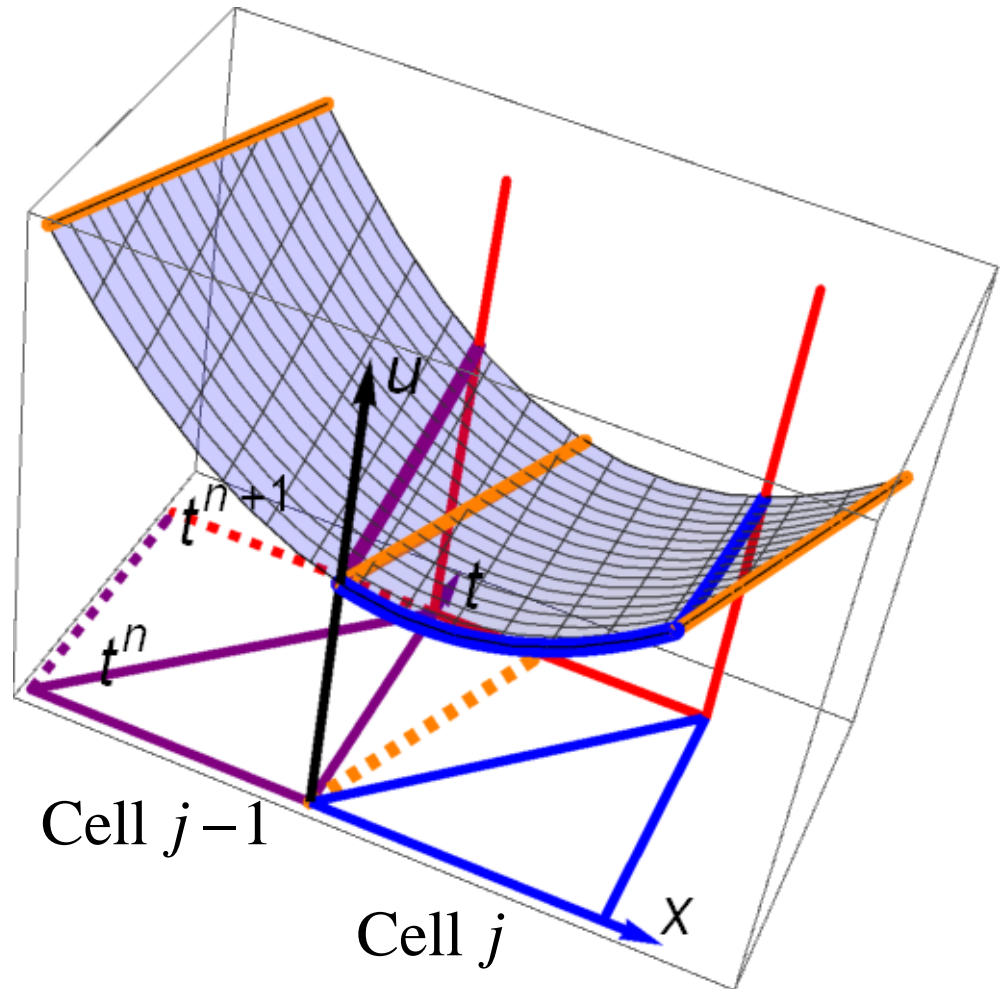
With u_j^n, $(u_x)_j^n$,

$(u_{xx})_j^n, \ldots$ known,

1. Obtain mixed derivatives

$u_t = -a u_x$,

$u_{xt} = -a u_{xx}, \ldots$

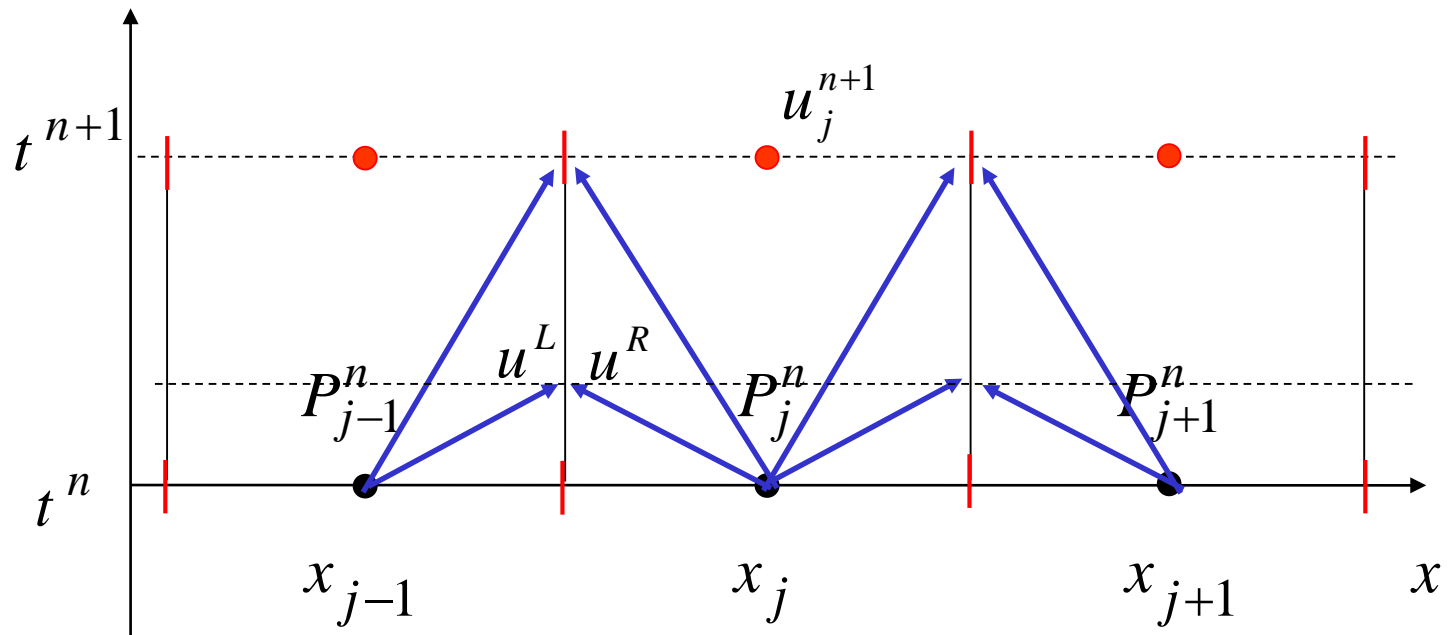via a Cauchy - Kowalewsky procedure (Harten Engquist, Osher, and Chakravarthy, 1987)
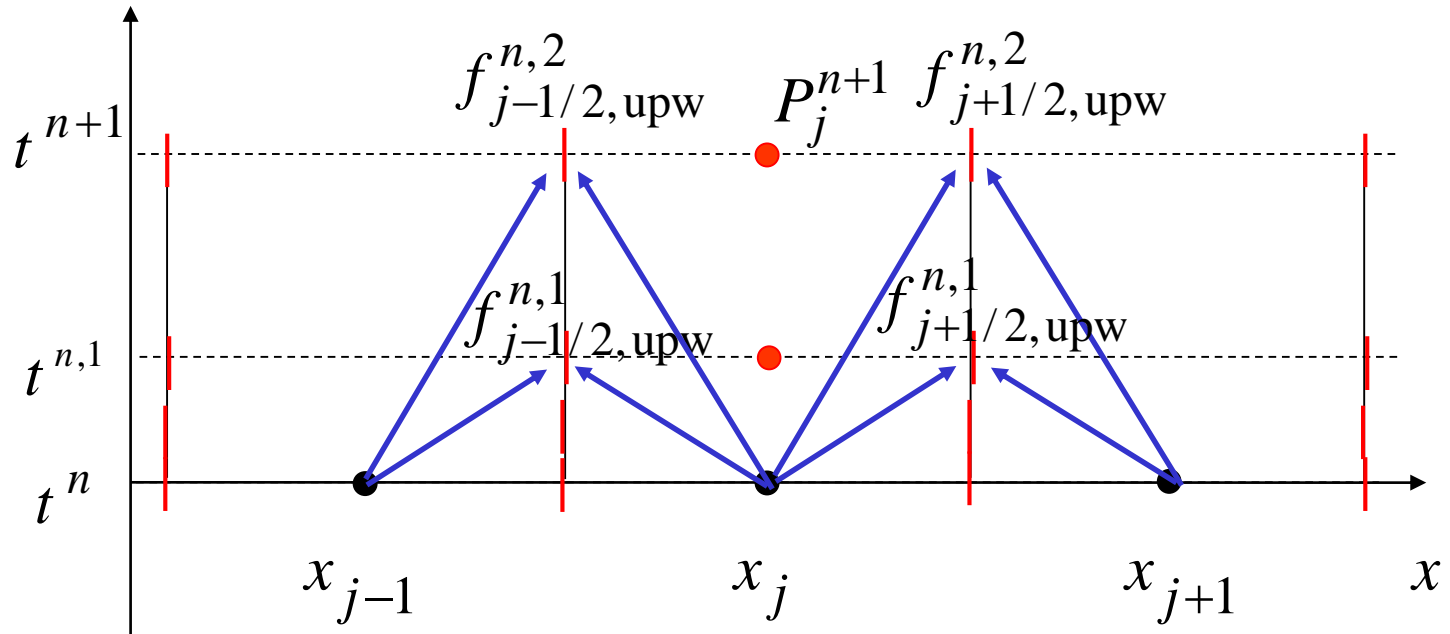
2. Or use Runge - Kutta with no upwinding.

We need to allow the data among cells to interact

Obtain Surface Fluxes at Radau Time Levels

At each interface, for each Radau time level,

with u_L and u_R known via, e.g., a C‑K procedure,

the flux is evaluated by upwinding (Riemann solver)

Update cell average values at red dots

$$\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t^*) L_k \, dx = \int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t^n) L_k \, dx -$$

$$\int_{t^n}^{t^*} [f_{\text{upw}} L_k]_{x_{j-1/2}}^{x_{j+1/2}} \, dt + \int_{t^n}^{t^*} \int_{x_{j-1/2}}^{x_{j+1/2}} (f)(L_k)_x \, dx \, dt$$
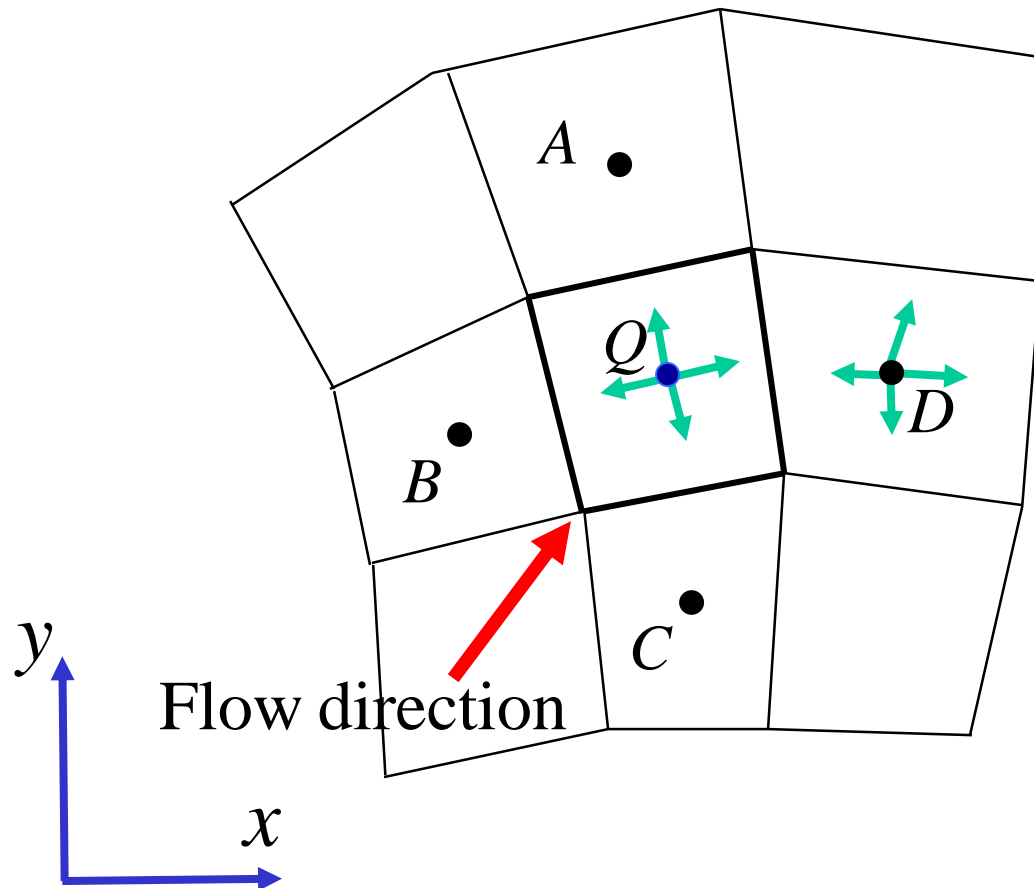
Algorithm for Moment Scheme

The piecewise polynomial data are given at time n.

- First, on each cell, obtain the space-time Taylor series expansion with no interaction (via Cauchy-Kovalevsky or RK)

- At each interface, for each Radau intermediate time level, get the left and right u values, and then the upwind fluxes.

- Successively calculate $u_{j,0}^{n,l}$, $u_{j,1}^{n,l}$, $u_{j,2}^{n,l}$, …
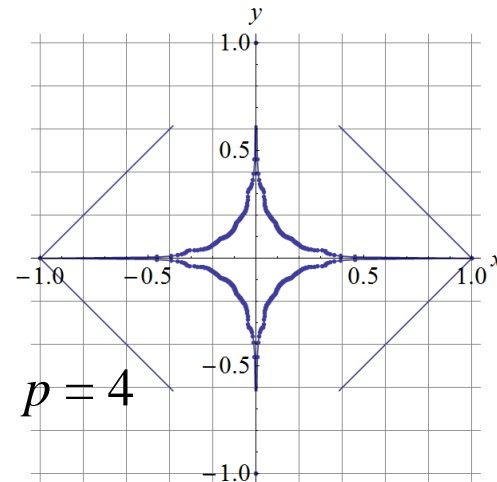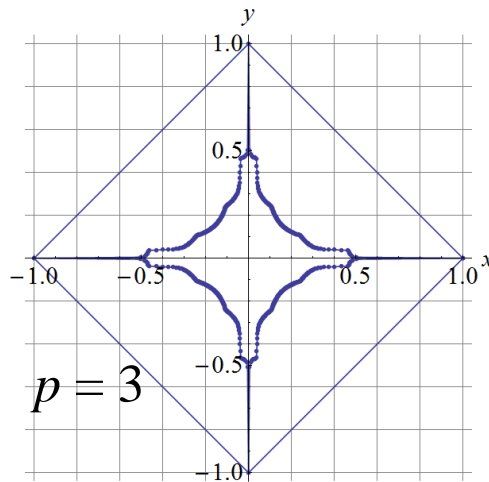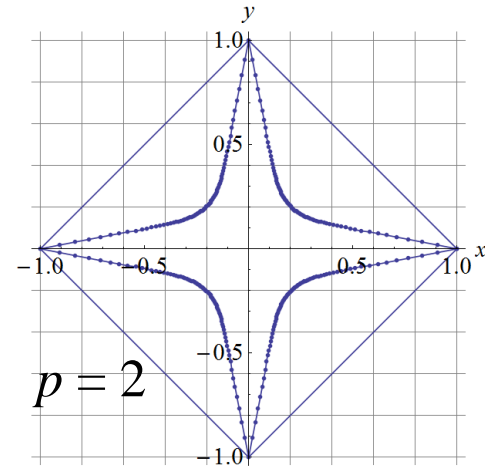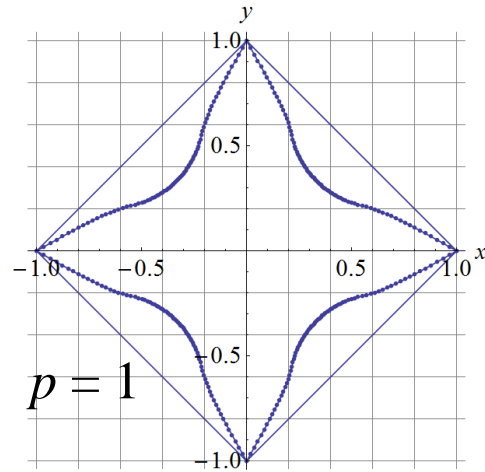
Moment Scheme (1D)

- For 1D convection with a constant speed, the moment scheme yields a result identical that via Van Leer's approach (accurate to order $2p + 1$).

- For a vanishingly small time step, the moment scheme reduces to RK-DG.

- The moment scheme extends to systems of equations with relative ease.

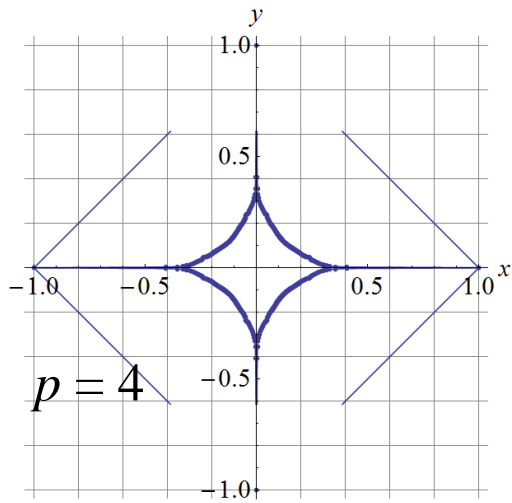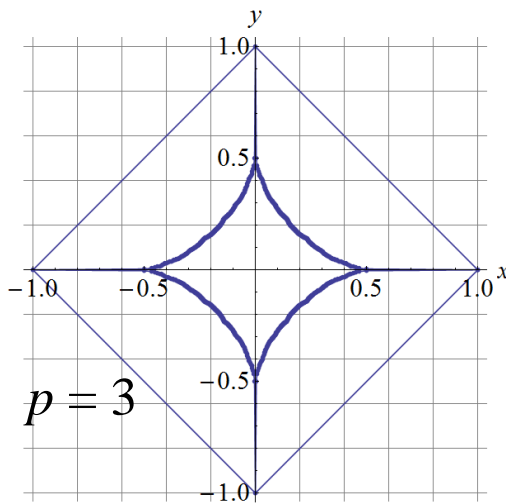# Moment Scheme on a Rectangular Mesh: Interacts with the four immediate neighbors
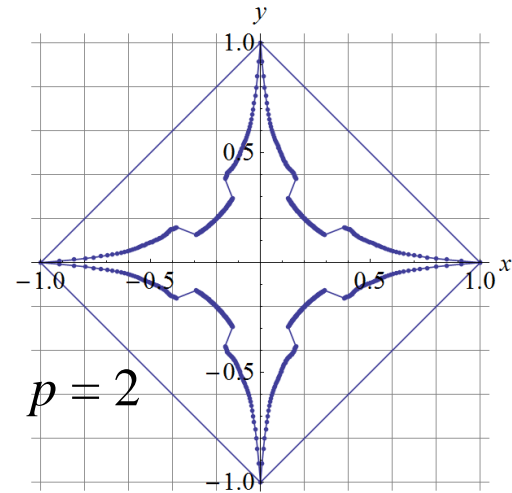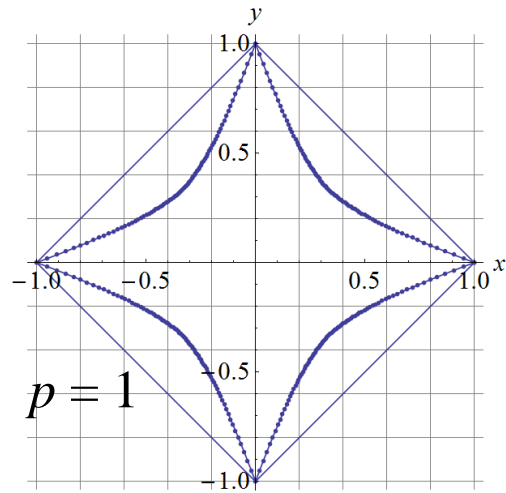
But does NOT involve corner neighbors

Flow direction

y

x

2D Fourier Analysis for Moment Scheme: Stability Regions

2D Fourier Analysis for Moment Scheme: Stability Regions, Tensor Products

Space-Time DG (Implicit) Method

On the (x,t) plane, set $\nabla = \left(\dfrac{\partial}{\partial x}, \dfrac{\partial}{\partial t} \right)$, $\quad (u, \phi) = \int_K u\,\phi\,dx\,dt$,
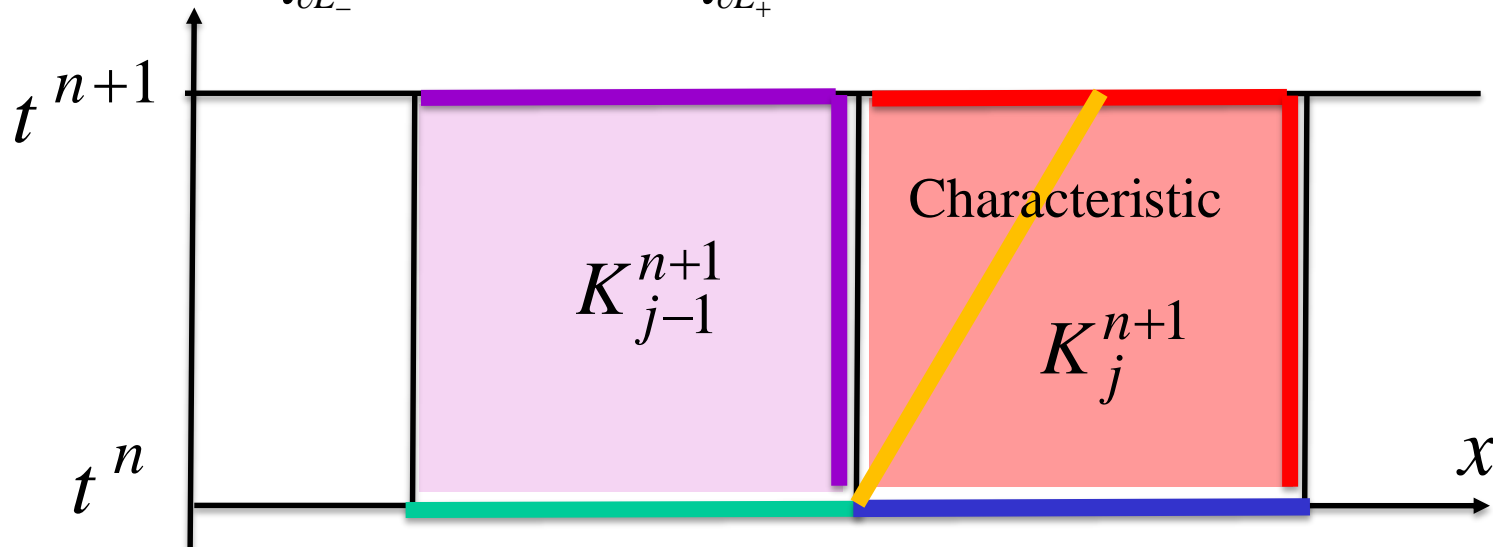
$$\beta = (a, 1), \quad u_\beta = \beta.\nabla u = a\,u_x + u_t.$$

Wish to solve $u_\beta = 0$. Using integration by parts,
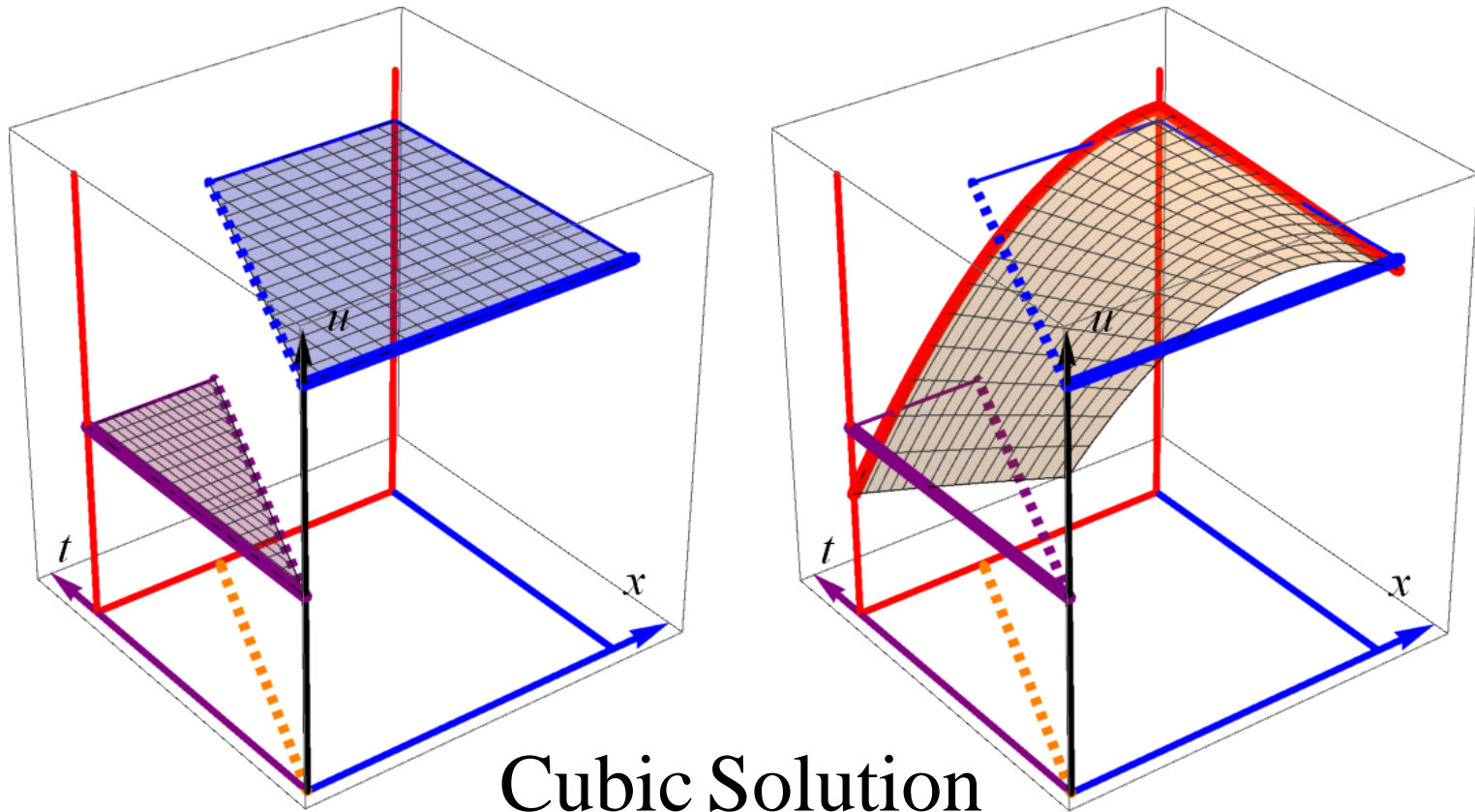
$$(u_\beta, \phi) = \int_{\partial E} u\,\phi\; n.\beta\,ds - (u, \phi_\beta) = 0$$

On domain K, find u_h of degree p such that for any ϕ of degree p,

$$\int_{\partial E_-} u_{\text{inflow}}\;\phi\; n.\beta\,ds + \int_{\partial E_+} u_h\,\phi\; n.\beta\,ds + (u_h, \phi_\beta) = 0.$$

t^{n+1}

t^n

K_{j-1}^{n+1}
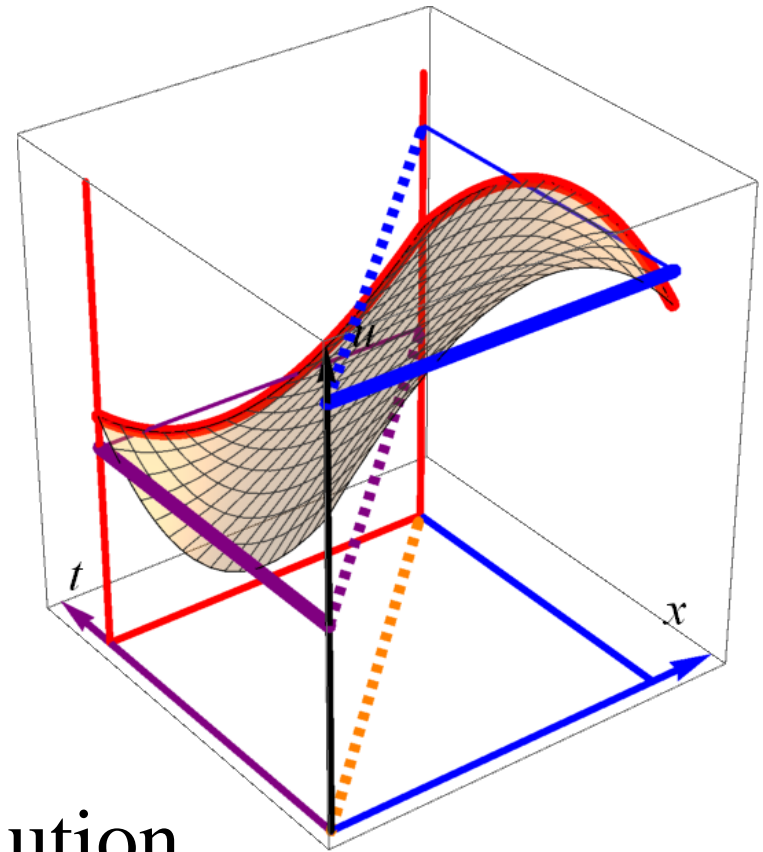
K_j^{n+1}

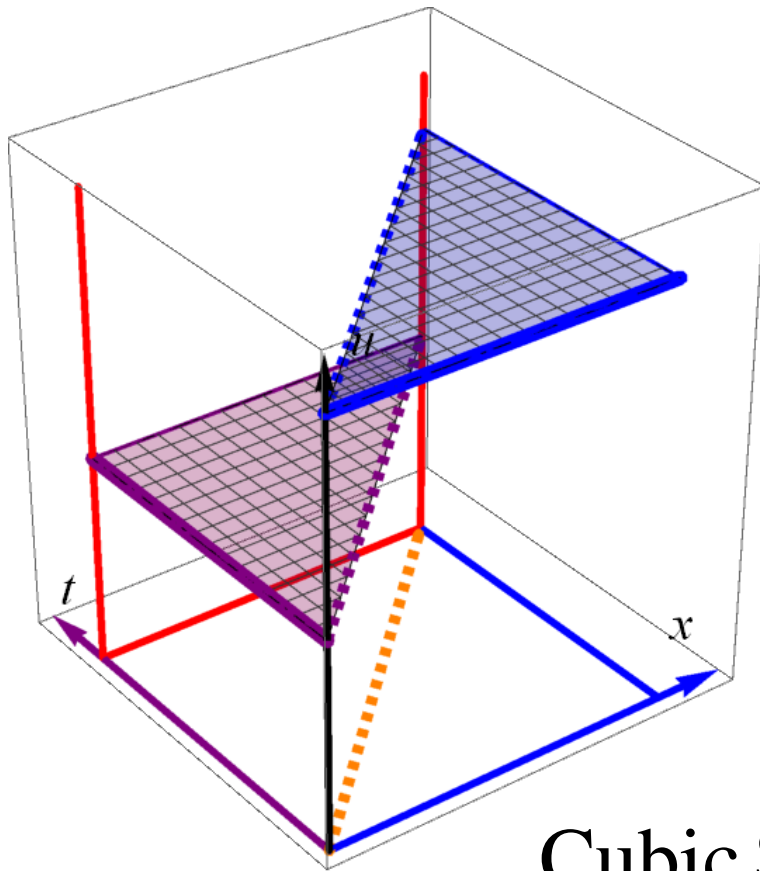Characteristic

x

Space-Time DG (Implicit) Method

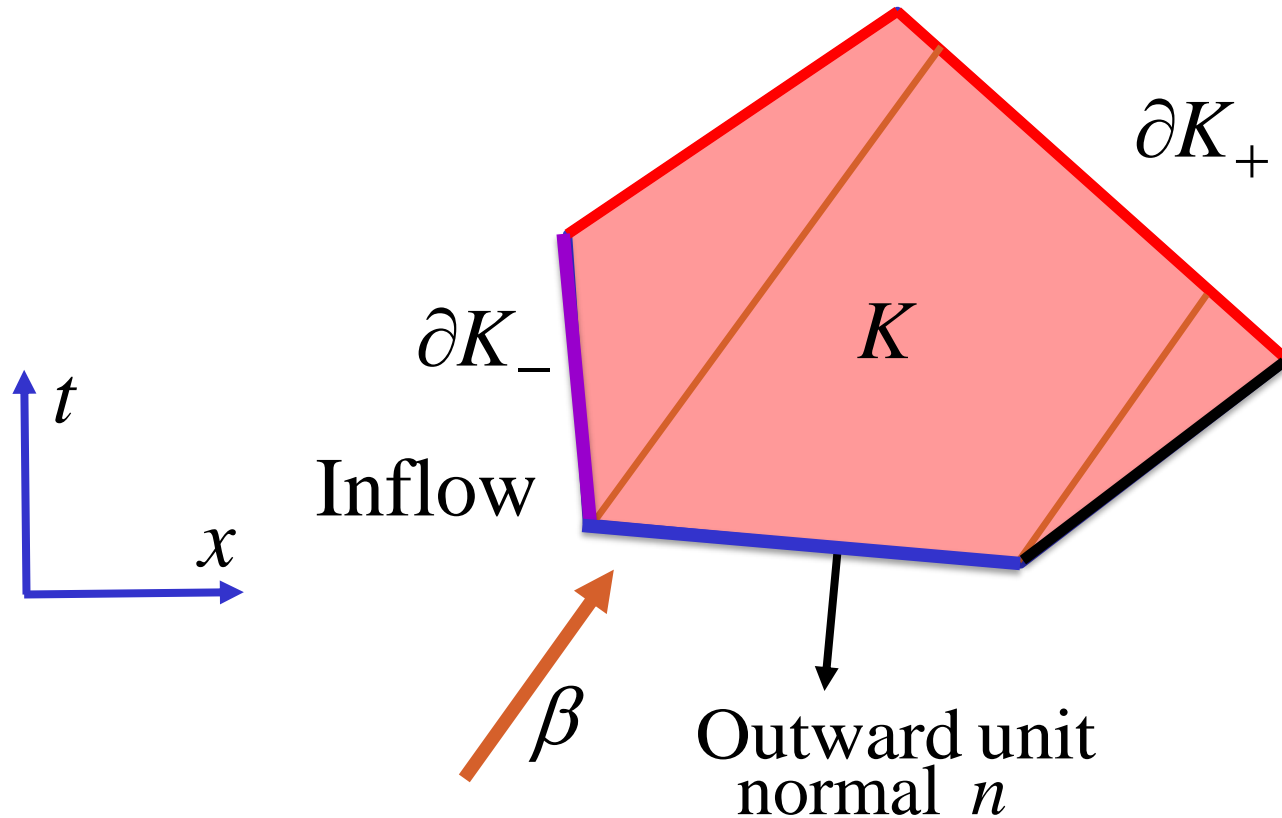Cubic Solution

$\sigma = 0.4$

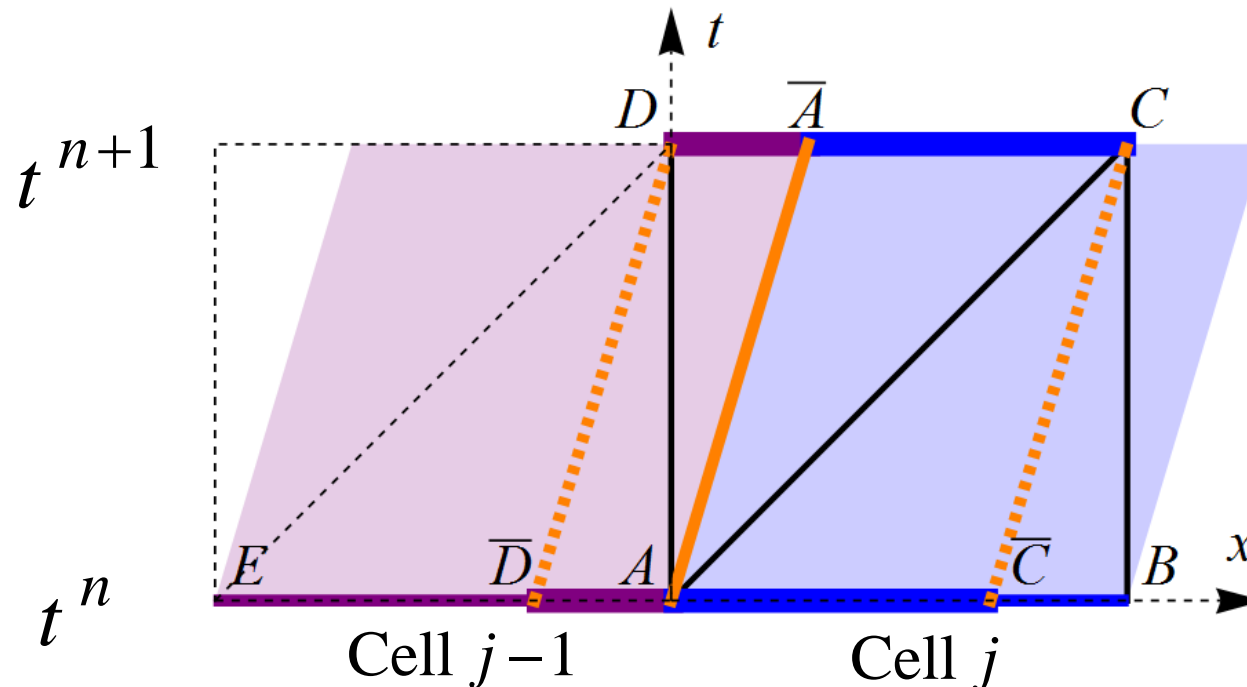# Space-Time DG (Implicit) Method

Cubic Solution

$$\sigma = 1$$

Space-Time Finite Element Method

$$\int_{\partial K_-} u_{\text{inflow}} \, \phi \, n.\beta \, ds \; + \; \int_{\partial K_+} u_h \, \phi \, n.\beta \, ds \; + \; (u_h, \phi_\beta) = 0.$$

Space-Time Finite Element Explicit Method for Advection
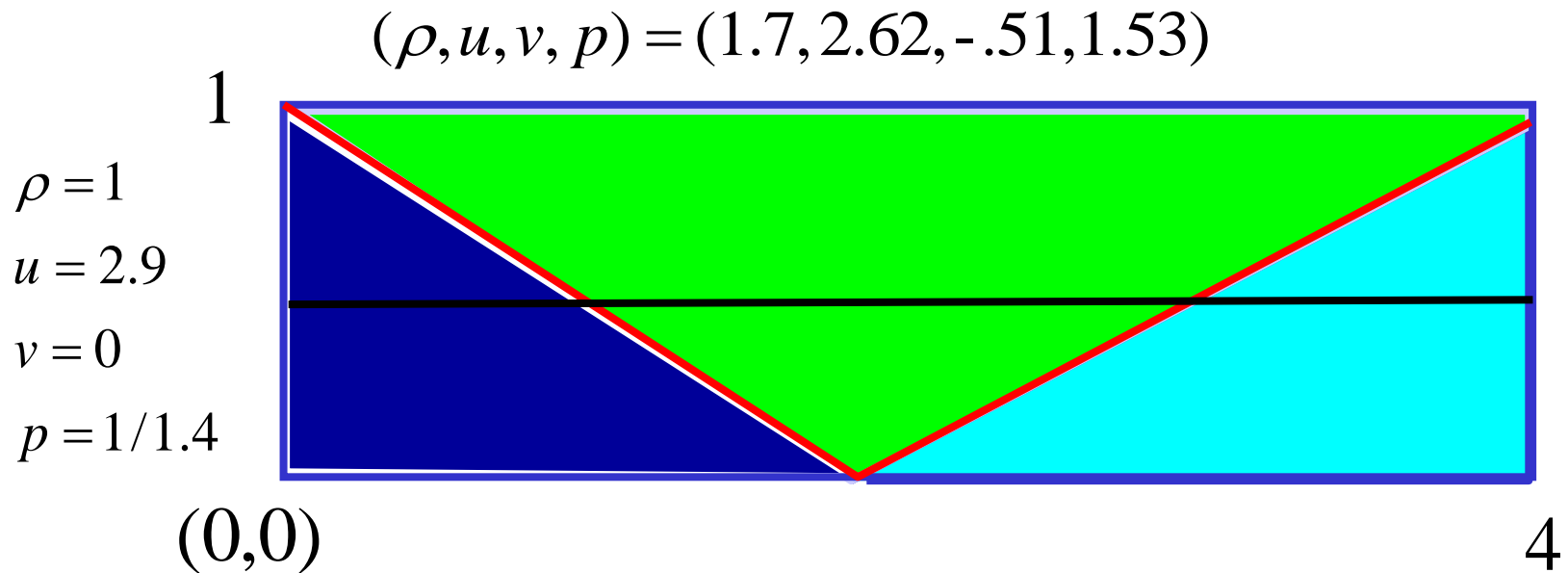
- Johnson and Pitkäranta 1986.

- Assume that $0 \leq \sigma \leq 1$.

- Triangulate each space-time cell by the diagonal from SW to NE.

- The solution is identical to that of Van Leer's method (FV=FE).

- Moment scheme provides extension for this explicit scheme to systems.

Moment Scheme and STDG

- STDG is not as accurate as the moment scheme, but is stable for arbitrary time step size.

- The solution expression for both method are the same except that the fluxes for the moment scheme are calculated explicitly from the data whereas those for STDG are implicit from the solutions.

- Van the moment scheme be employed in some iterative manner to obtain the solution of STDG without solving a large system of equations?
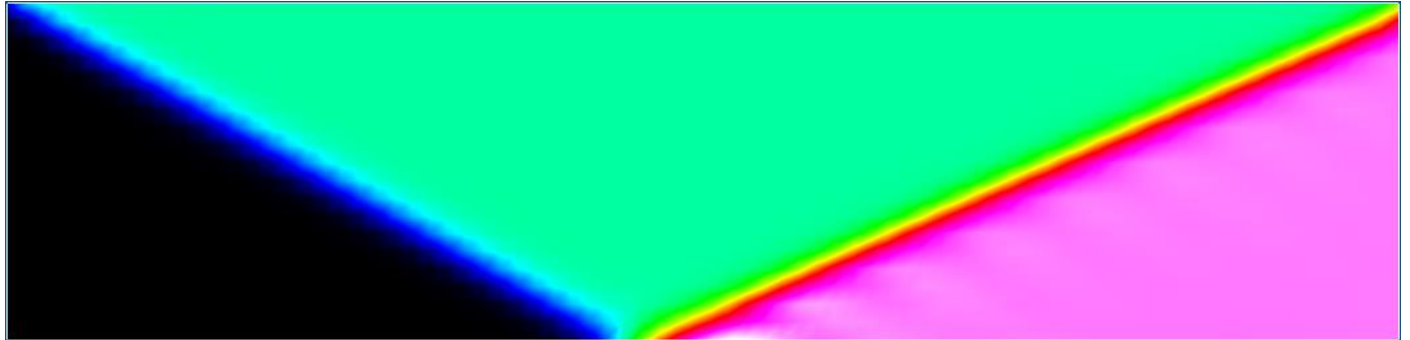
Oblique shock

$$(\rho, u, v, p) = (1.7, 2.62, -.51, 1.53)$$

$\rho = 1$

$u = 2.9$

$v = 0$
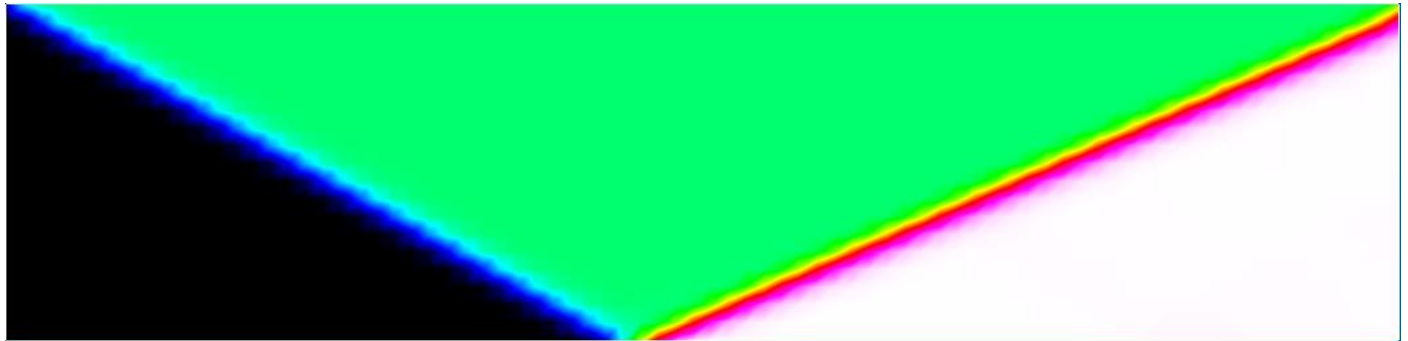
$p = 1/1.4$

1

(0,0)

4

Pressure

Upwind

Linear
Moment
Scheme

Conclusions

- A new idea for time stepping taking into account the physics of advection was presented. The method is an explicit time stepping with a CFL number of 1 in 1D.

- Moment schemes are (super) accurate to order $2p+1$.

- The implicit method is a simplified and optimal DG scheme applied to time. It employs the right Radau points.

- The explicit and implicit methods use the same intermediate time levels, and the former can serve as an iterative procedure to update the solution of the latter.

- Preliminary numerical results were shown.

- Further research on both type of time-stepping methods is needed.