A Kinetic Scheme for Gas Dynamics on Arbitrary Grids

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Agenda

- Finite volume discretizations & meshing strategies.
- The small cell problem.
- A kinetic scheme solving the problem!
- Numerical results.
- Future directions.

1D Euler Equations

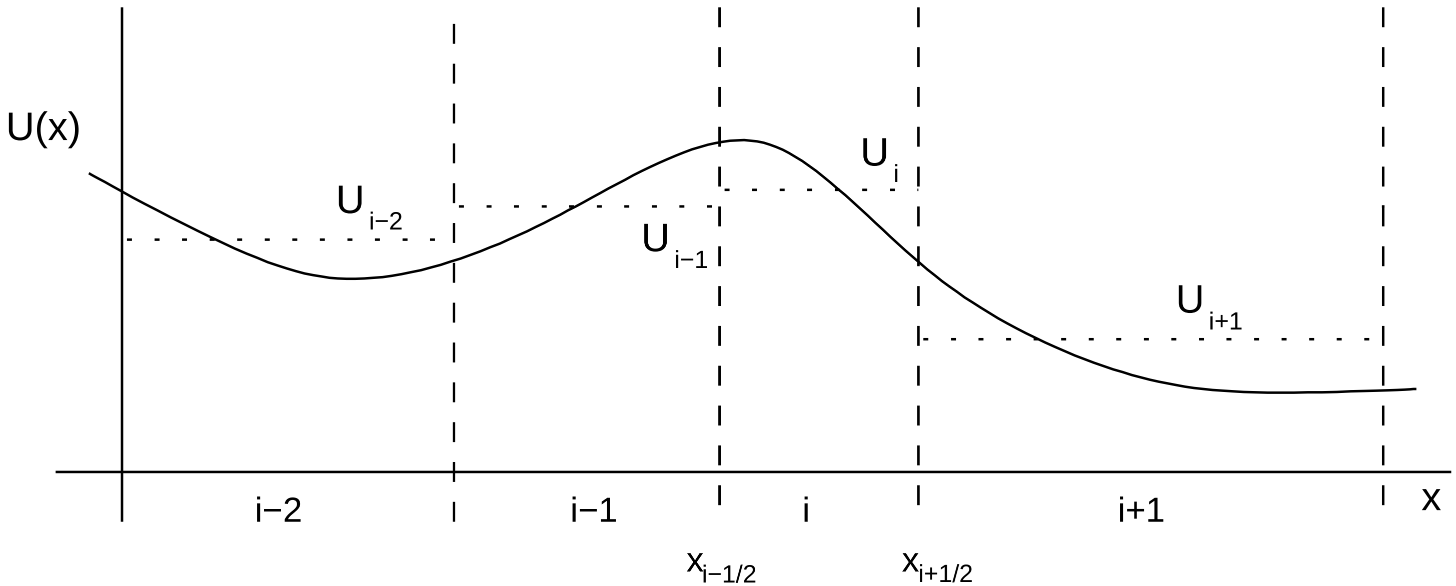
$$\begin{pmatrix} \rho \\ \rho u \\ \rho e \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (\rho e + p)u \end{pmatrix}_x = 0$$

- In the form $\mathbf{U}_t + \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{U}) = 0$
- Solutions develop discontinuities requiring special treatment — conservative schemes, non-oscillatory interpolation
- Finite wave speed $\Longrightarrow$ explicit schemes for time-accurate solutions
- Conservation law $\Longrightarrow$ finite volume discretization

Finite volume discretization

Finite volume discretization–store cell-averages:

$$\mathbf{U}_i^n = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x, t_n)\; dx.$$

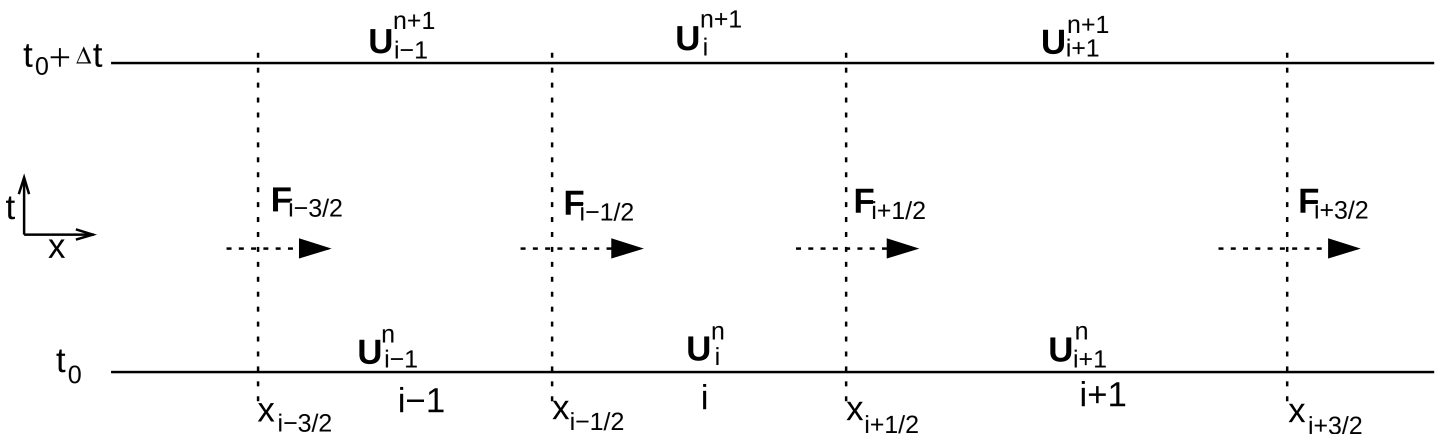


Integrating over $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [t_n, t_n + \Delta t]$ yields:

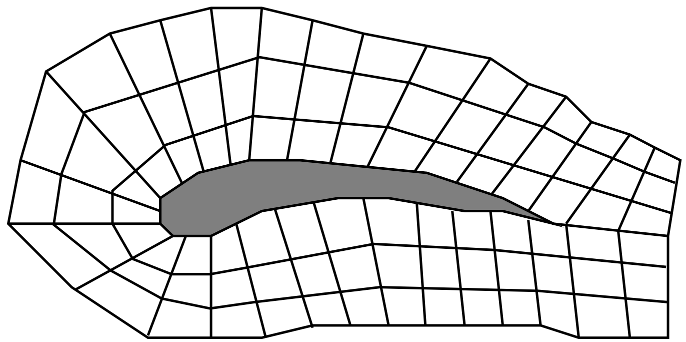
$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x_i}(\mathbf{F}_{i+1/2}^n - \mathbf{F}_{i-1/2}^n)$$

for time averaged flux

$$\mathbf{F}_{i\pm 1/2}^n = \frac{1}{\Delta t} \int_{t_n}^{t_n+\Delta t} \mathbf{F}\big(\mathbf{U}(x_{i\pm 1/2}, t)\big)\, dt$$

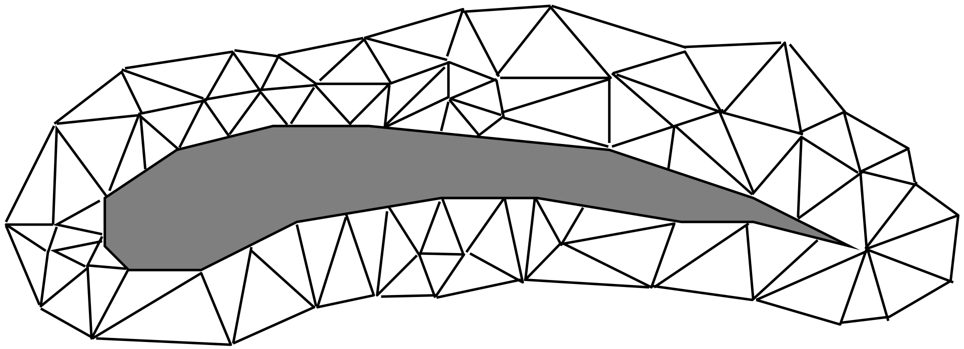


Body-fitted Structured Mesh



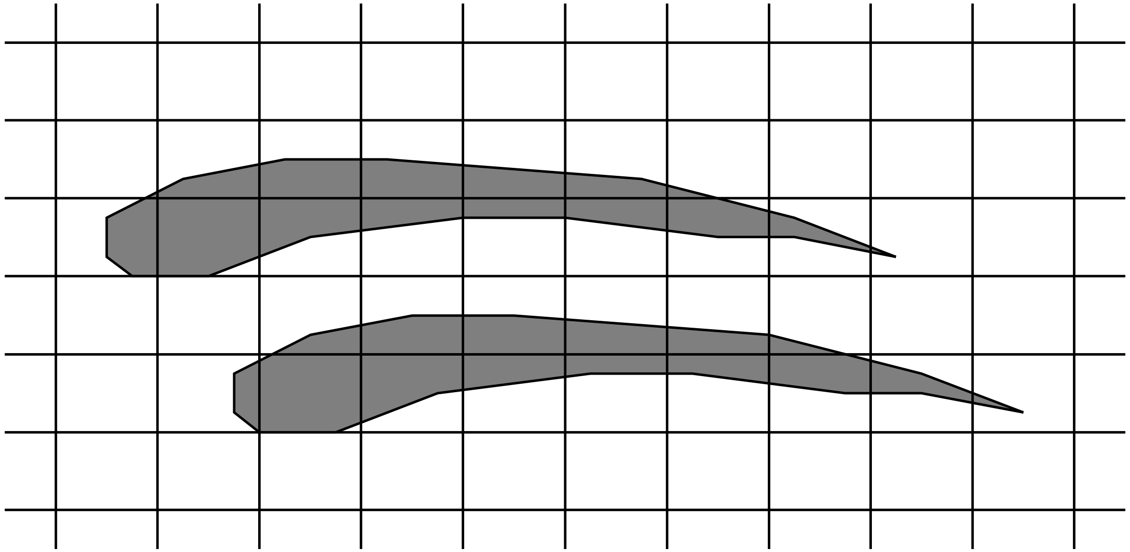
Easy to write operators for but very difficult to generate for complicated domains.

Unstructured Mesh



Operators have to carry grid connectivity information; load balancing issues.

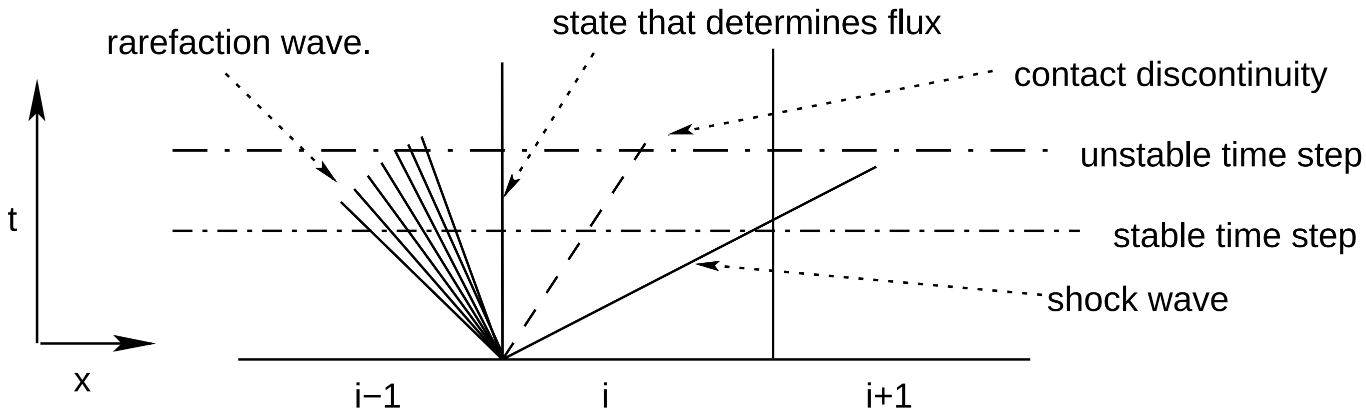
Cartesian Mesh



Amenable to automatic generation, good for parallelization, but has irregular arbitrarily small cells near boundary.

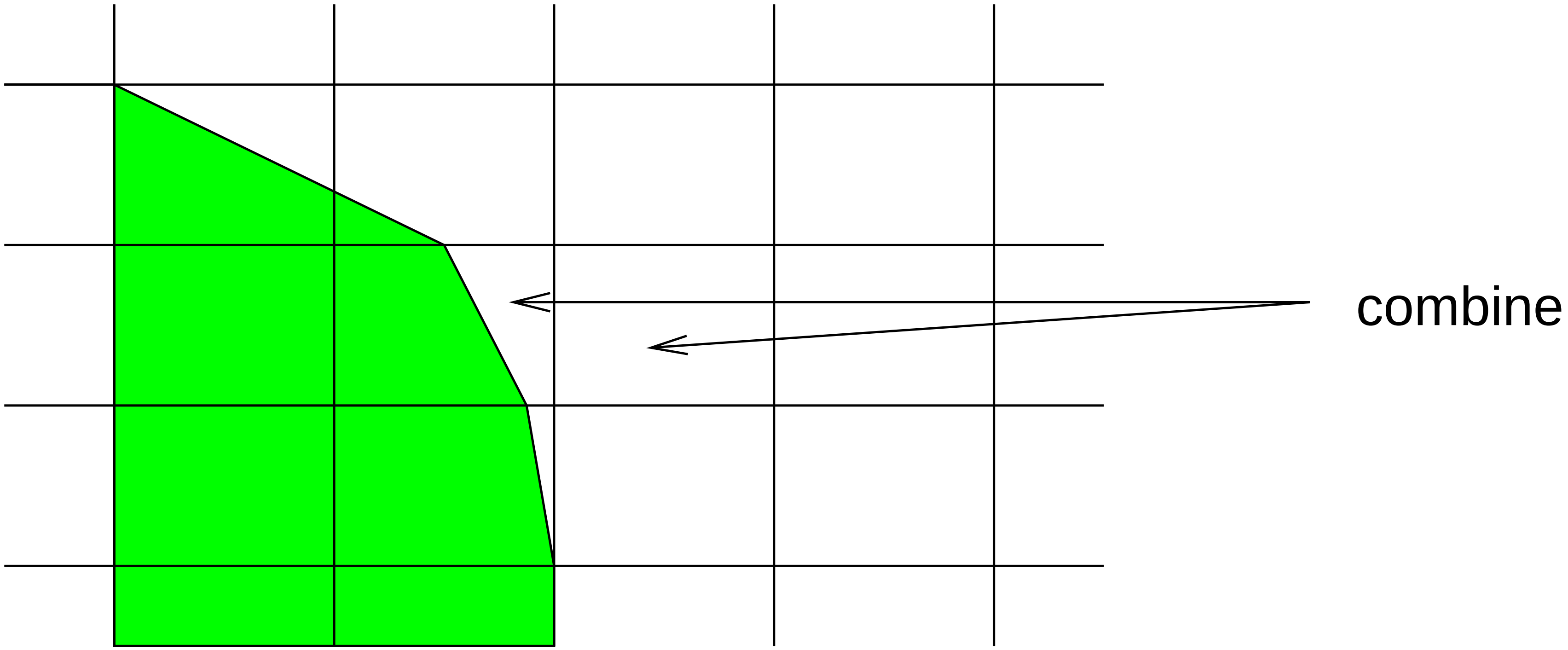
CFL and the Small Cell Problem

- Flux $\mathbf{F}_{i+\frac{1}{2}}$ comes from solving local IVP (Riemann problem) on the face.
- Waves from nearby faces must not reach other faces during a timestep - *domain of dependence of a face must be within adjacent cells.*



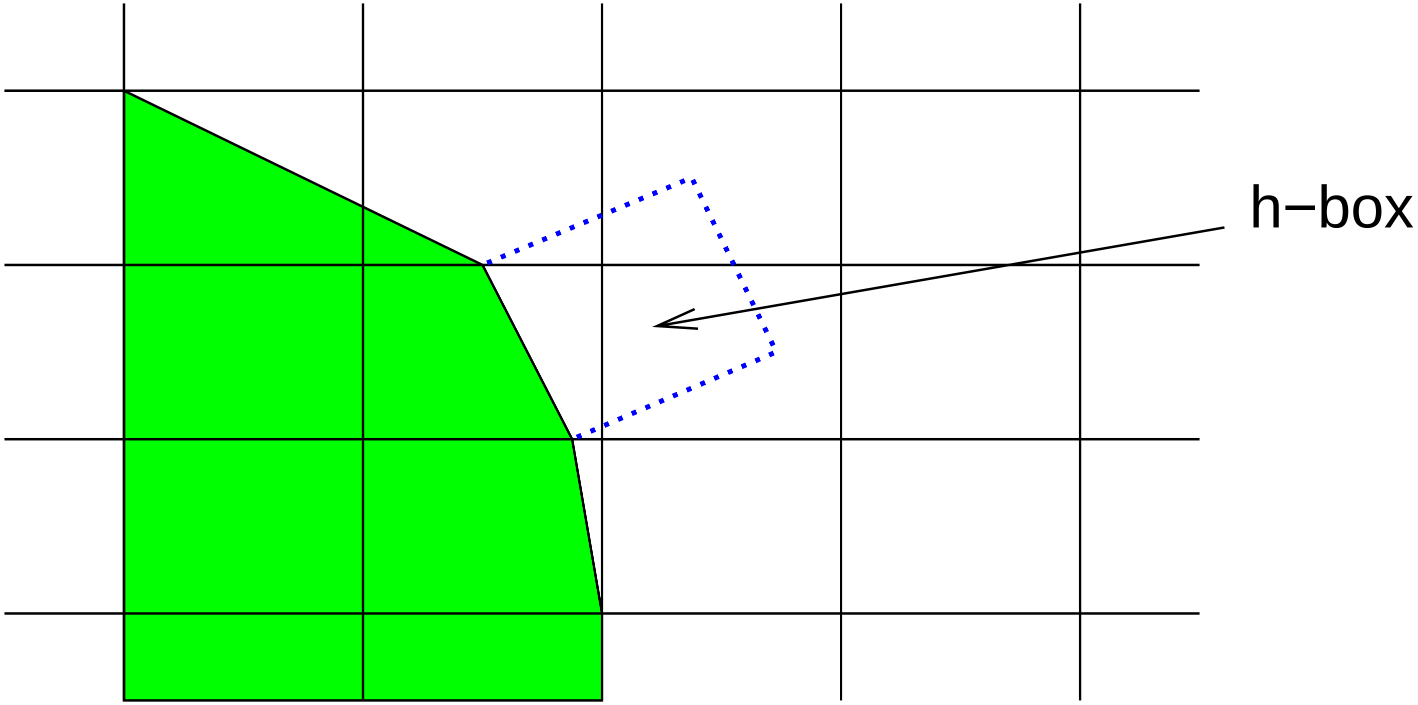
- Therefore $\Delta t = O(\Delta x_i)$—unacceptable for Cartesian meshes.

Existing Approaches



Cell Merging

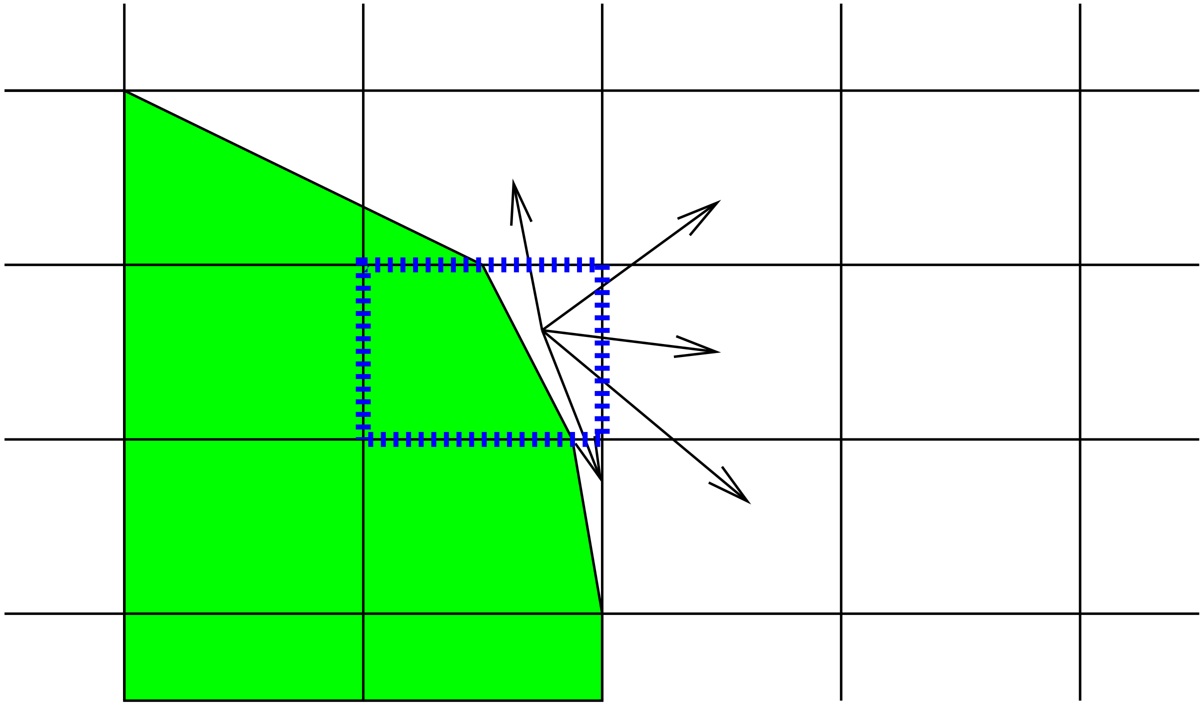
Quirk 1994; Coirier and Powell 1995; Hunt 2004



O(h)-boxes

Berger and LeVeque 1990;

Helzel, Berger, and LeVeque 2003



Flux Redistribution

Pember, Bell, Colella, Crutchfield, Welcome ’95;

Modiano and Colella 2000

Kinetic Frameworks

- Boltzmann equation: *non-equilibrium* gas dynamics via particle density $f(\mathbf{x}, \mathbf{v}, t)$ in phase space:

$$f_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f)$$

- Fluid quantities are moments of particle density, e.g:

$$\rho(\mathbf{x}, t) = \int_{\mathbb{R}^n} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$

- In fluid limit (mean free path $\to 0$)
  Boltzmann solution $\to$ Euler solution
- Strategy for a time step:
  - define density distribution f from fluid state $\mathbf{U}$
  - evolve according to approximation of Boltzmann
  - take moments to recover new fluid state, cell average.

Kinetic Scheme (Perthame 1992, 1994)

- Notation for 1D construction:
  - temperature $T = p/\rho$; $w = (v-u)/\sqrt{T}$
  - $\chi(x) = (2\sqrt{3})^{-1}$ if $|x| < \sqrt{3}$, 0 otherwise.
- Given $\mathbf{U}(x,0)$, define initial distributions:

$$f_0(x;v) = \frac{\rho_0(x)}{\sqrt{T_0(x)}}\chi(w(x))$$

$$g_0(x;v) = \lambda\rho_0(x)\sqrt{T_0(x)}\chi(w(x))$$

- Use this as initial condition in *collisionless* transport:

$$f_t + vf_x = 0, \quad g_t + vg_x = 0$$

- Define the fluid state implied by the transport:

$$\widetilde{\mathbf{U}}(x,t) = \int\limits_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ v^2/2 \end{pmatrix} f_0(x - vt; v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_0(x - vt; v)\ dv;$$

note $\widetilde{\mathbf{U}}(x,0) = \mathbf{U}(x,0)$.

- Further, note

$$\int\limits_{\mathbb{R}} \begin{pmatrix} v \\ v^2 \\ v^3/2 \end{pmatrix} f_0(x; v) + \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix} g_0(x; v)\ dv = \mathbf{F}\big(\mathbf{U}(x,0)\big)$$

- By comparing Taylor expansions in t,

$$\widetilde{\mathbf{U}}(x,\Delta t) = \mathbf{U}(x,\Delta t) + O(\Delta t^2).$$

Scheme Properties

- Effect of collision via projecting $f; g$ back to fluid state $\mathbf{U}$.
- L_1**-stable;** $\rho(x,t),\ T(x,t) \geq 0$ **pointwise positive.**
- **No restriction on** Δt **if transport solved exactly.**
- Second order by modifying initial distributions:

- For a cell $\mathcal{T}_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$:

$$\Delta x_i \mathbf{U}_i(\Delta t) = \int\limits_{\mathcal{T}_i}\int\limits_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f(x,v,\Delta t) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g(x,v,\Delta t)\ dv\ dx$$

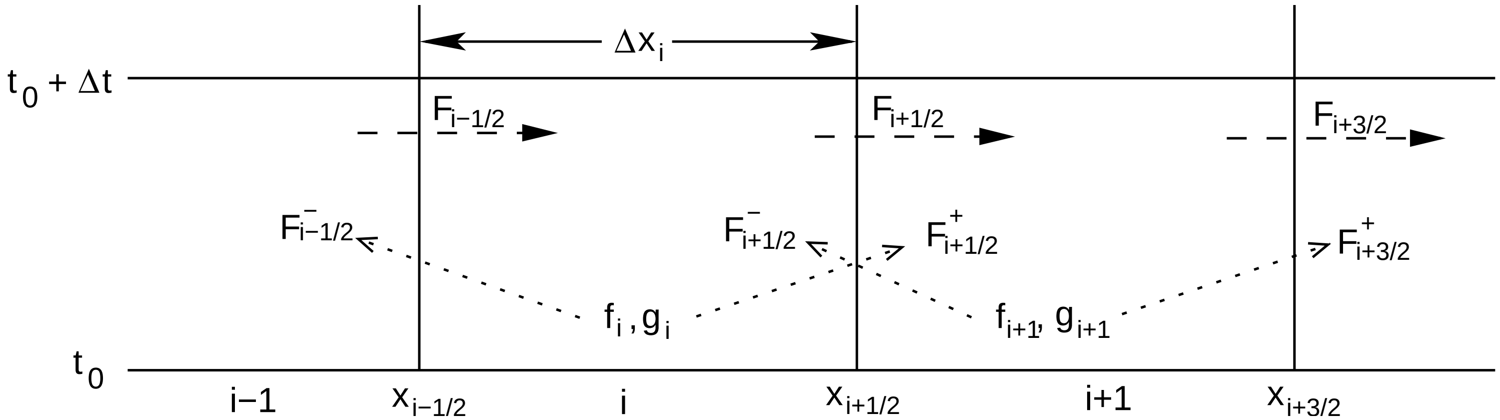
$$= \Delta x_i \mathbf{U}_i(0) + \int\limits_0^{\Delta t}\int\limits_{\mathbb{R}} \begin{pmatrix} v \\ v^2 \\ \frac{v^3}{2} \end{pmatrix} f(x_{i-\frac{1}{2}},v,t) + \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix} g(x_{i-\frac{1}{2}},v,t)\ dv\ dt$$

$$- \int\limits_0^{\Delta t}\int\limits_{\mathbb{R}} \begin{pmatrix} v \\ v^2 \\ \frac{v^3}{2} \end{pmatrix} f(x_{i+\frac{1}{2}},v,t) + \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix} g(x_{i+\frac{1}{2}},v,t)\ dv\ dt.$$

- Flux: $\mathbf{F}_{i+\frac{1}{2}} = \mathbf{F}^-_{i+\frac{1}{2}} + \mathbf{F}^+_{i+\frac{1}{2}}$ — leftward and rightward moving particles.

$$\mathbf{F}^+_{i+\frac{1}{2}} = \int\limits_0^{\Delta t}\int\limits_{v>0} \begin{pmatrix} v \\ v^2 \\ \frac{v^3}{2} \end{pmatrix} f_i(x_{i+\frac{1}{2}} - v\Delta t; v) + \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix} g_i(x_{i+\frac{1}{2}}, -v\Delta t; v)\ dv\ dt$$

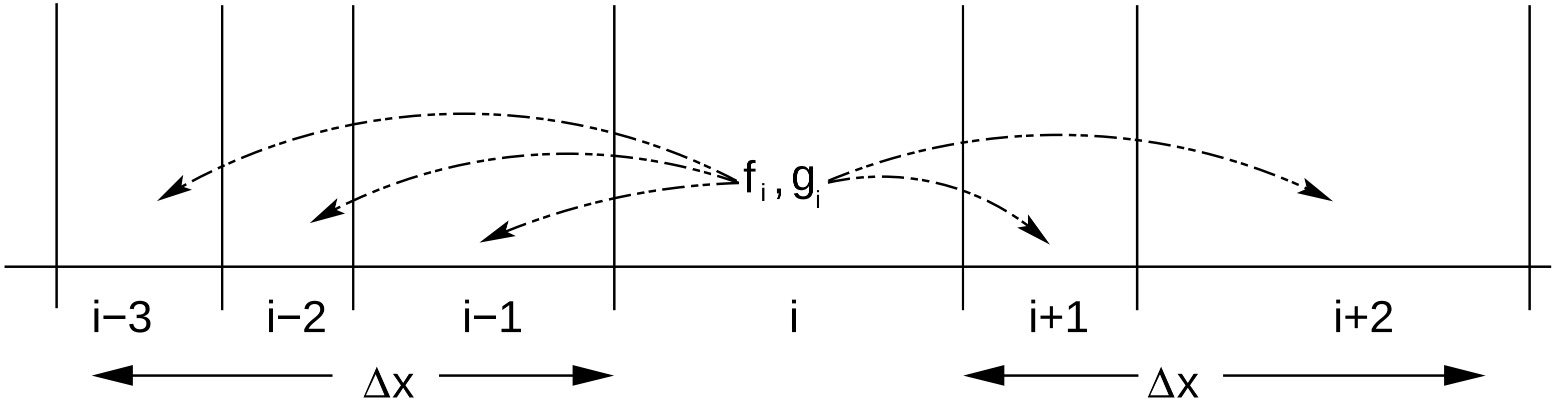
CFL Redux: Flux Formulation



- Flux formula depends only on adjacent cells
- CFL restriction for the transport equation!
- Max particle speed $v_{\rm max}$, timestep Δt, min cell size $\Delta x_{\rm min}$ must satisfy

$$\Delta t \; v_{\rm max} < \Delta x_{\rm min}$$

Direct Transport Formulation



$$\Delta x_i \mathbf{U}_i(\Delta t) = \Delta x_i \mathbf{U}_i(0)$$

$$+\sum_{j\neq i}\int_{\mathcal{T}_i}\int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f_j(x - v\Delta t; v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_j(x - v\Delta t; v)\ dv\ dx$$

$$-\sum_{j\neq i}\int_{\mathcal{T}_j}\int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f_i(x - v\Delta t; v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_j(x - v\Delta t; v)\ dv\ dx$$

CFL constraint vanishes; unconditionally stable explicit scheme. . .

- *Choose* domain of dependence Δx;
  corresponding Δt is *independent* of mesh size.

- Must compute transport from source cell $\mathcal{S}$ to target $\mathcal{T}$ during Δt; only targets within Δx considered, need not be adjacent.

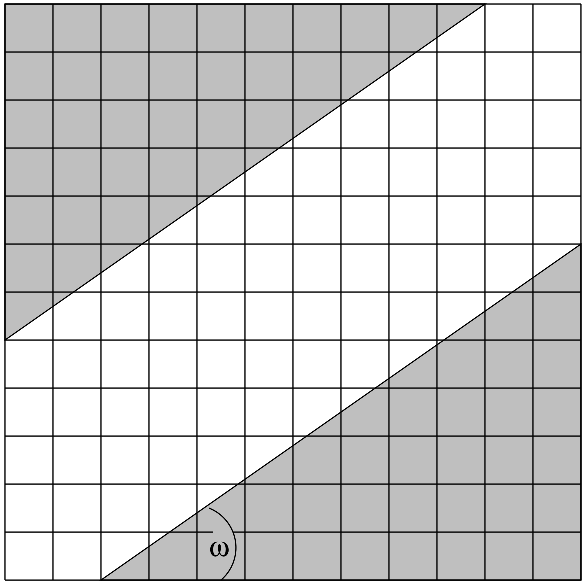
$$\int\limits_{x\in\mathcal{S}} \int\limits_{x+v\Delta t\in\mathcal{T}} \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f_0(x,v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_0(x,v) dv\ dx.$$

- Simple structure in v-space $\Longrightarrow$ practical to evaluate

- Extends to unsplit higher dimensional scheme.

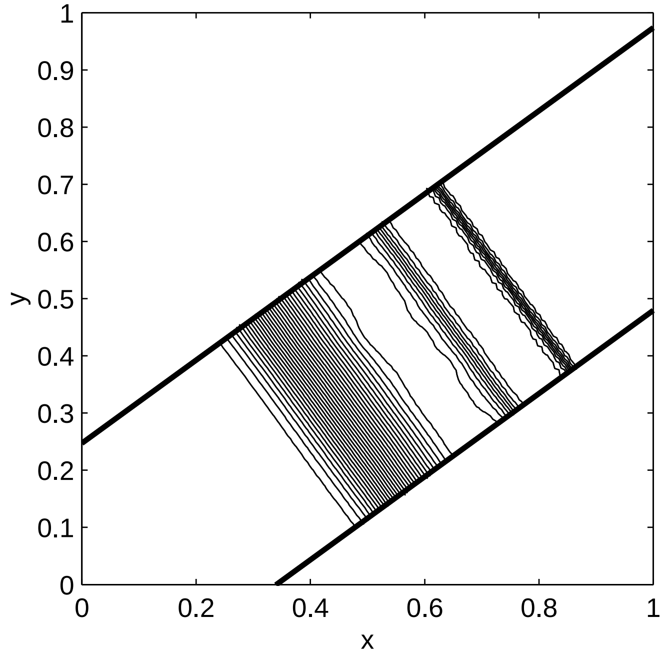
- *No degradation of accuracy or extra diffusion near small cells.*

Oblique Channel Flow



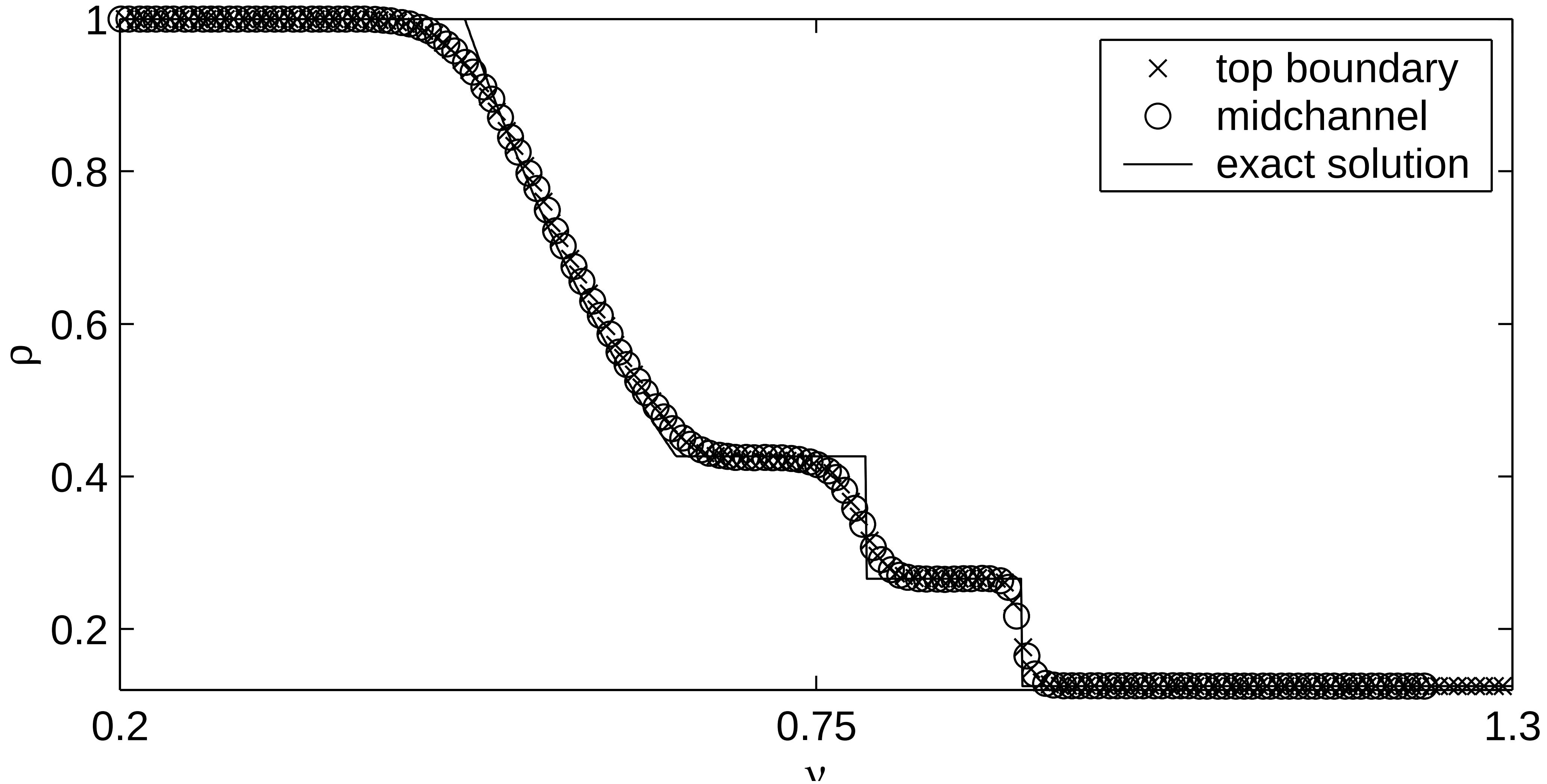
Allows study of the effect of the embedded boundary on channel aligned plane waves

Channel Aligned Sod Shock Tube



100x100 underlying mesh; 50 density contours at t=0.15

Channel Aligned Sod Shock Tube



Comparison of boundary and mid-channel solution

Channel Convergence Tests

Measure L_1, L_∞ convergence in the domain as a whole, and L_1 the cells within Δx of the boundary.

Channel Aligned Advection

C_0^∞ density perturbation ($\pm$ 8%):

$$(\rho_0(\mathbf{x}), u_1, u_2, p_0) = (2 + h(\mathbf{x}), \cos(\omega), \sin(\omega), 1),$$

where

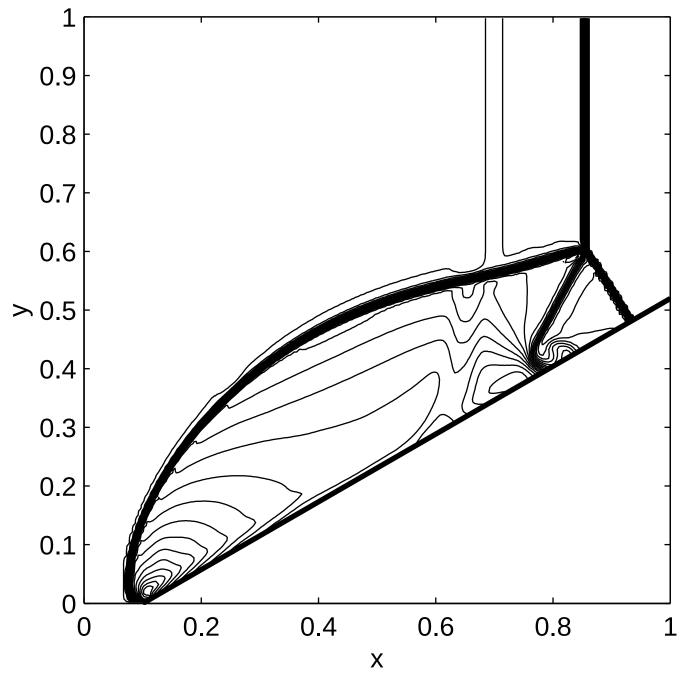
$$h(\mathbf{x}) = \begin{cases} 10\exp\Big(-\big((1.5-5\nu)(2.5-5\nu)\big)^{-1}\Big) & 0.3 < \nu < 0.5, \\ 0 & \text{otherwise.} \end{cases}$$

and ν is the coordinate aligned with the channel; solve to $t = 0.2$.

Channel Aligned Advection

Δx	$\|e\|_1$	$k(L_1)$	$\|e\|_{1,\partial}$	$k(L_{1,\partial})$	$\|e\|_\infty$	$k(L_\infty)$
2^{-6}	5.28e-3		8.62e-5		1.15e-2	
2^{-7}	1.10e-4	**2.26**	9.24e-6	**2.22**	3.23e-3	**1.83**
2^{-8}	2.2e-5	**2.32**	9.26e-7	**2.32**	7.63e-4	**2.08**
2^{-9}	4.55e-6	**2.27**	1.05e-7	**2.14**	2.05e-4	**1.90**

Oblique shock reflection



- 200x200 underlying mesh; $\omega = \pi/6$; 50 density contours at t=0.22
- M=2.87; smallest cell is 2.3×10^{-5} regular volume

Summary of Results

- Unconditionally stable explicit scheme - no small cell problem on Cartesian meshes
- Everywhere conservative and second order accurate
- Proven to be L_1 stable and positive in density and internal energy.

Extensions

- 3 space dimensions, parallel implementation, grid adaption
- Boundary conditions, moving boundaries