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

\[
\begin{pmatrix}
\rho \\
\rho u \\
\rho e
\end{pmatrix}
+ \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
(\rho e + p)u
\end{pmatrix} = 0
\]

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

Finite volume discretization–store cell-averages:

\[
U^n_i = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t_n) \, dx.
\]
Integrating over \([x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [t_n, t_n + \Delta t]\) yields:

\[
U_{i}^{n+1} = U_{i}^{n} - \frac{\Delta t}{\Delta x_i} (F_{i+1/2}^{n} - F_{i-1/2}^{n})
\]

for time averaged flux

\[
F_{i \pm 1/2}^{n} = \frac{1}{\Delta t} \int_{t_n}^{t_{n+\Delta t}} F(U(x_{i \pm 1/2}, t)) \, dt
\]
Body-fitted Structured Mesh

Easy to write operators for but very difficult to generate for complicated domains.
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 $F_{i+\frac{1}{2}}$ 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
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 $f(x, v, t)$ in phase space:
  \[ f_t + v \cdot \nabla_x f = Q(f, f) \]

- Fluid quantities are moments of particle density, e.g:
  \[ \rho(x, t) = \int_{\mathbb{R}^n} f(x, v, t) dv \]

- In fluid limit (mean free path $\rightarrow 0$)
  Boltzmann solution $\rightarrow$ Euler solution

- Strategy for a time step:
  - define density distribution $f$ from fluid state $U$
  - 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 $U(x, 0)$, 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 \textit{collisionless} transport:

  $$f_t + vf_x = 0, \quad g_t + vg_x = 0$$
Define the fluid state implied by the transport:

\[ \tilde{U}(x, t) = \int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ v^2/2 \end{pmatrix} f_0(x - vt; v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_0(x - vt; v) \, dv; \]

note \( \tilde{U}(x, 0) = U(x, 0) \).

Further, note

\[ \int_{\mathbb{R}} \begin{pmatrix} v \\ v^2 \\ v^3/2 \end{pmatrix} f_0(x; v) + \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix} g_0(x; v) \, dv = F(U(x, 0)) \]

By comparing Taylor expansions in \( t \),

\[ \tilde{U}(x, \Delta t) = U(x, \Delta t) + O(\Delta t^2). \]
Scheme Properties

- Effect of collision via projecting $f;g$ back to fluid state $U$.
- $L_1$-stable; $\rho(x,t), T(x,t) \geq 0$ pointwise positive.
- No restriction on $\Delta t$ if transport solved exactly.
- Second order by modifying initial distributions:
• For a cell $T_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$:

$$
\Delta x_i U_i(\Delta t) = \int_{T_i} \int_{\mathbb{R}} \left( \frac{1}{v^2} \right) f(x, v, \Delta t) + \left( \begin{array}{c} 0 \\ 0 \end{array} \right) g(x, v, \Delta t) \ dv \ dx
$$

$$
= \Delta x_i U_i(0) + \int_0^{\Delta t} \int_{\mathbb{R}} \left( \begin{array}{c} v \\ v^2 \\ v^3 \\ v^4 \end{array} \right) f(x_{i-\frac{1}{2}}, v, t) + \left( \begin{array}{c} 0 \\ 0 \end{array} \right) g(x_{i-\frac{1}{2}}, v, t) \ dv \ dt
$$

$$
- \int_0^{\Delta t} \int_{\mathbb{R}} \left( \begin{array}{c} v \\ v^2 \\ v^3 \\ v^4 \end{array} \right) f(x_{i+\frac{1}{2}}, v, t) + \left( \begin{array}{c} 0 \\ 0 \end{array} \right) g(x_{i+\frac{1}{2}}, v, t) \ dv \ dt.
$$

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

$$
F^+_{i+\frac{1}{2}} = \int_0^{\Delta t} \int_{v>0} \left( \begin{array}{c} v \\ v^2 \\ v^3 \\ v^4 \end{array} \right) f_i(x_{i+\frac{1}{2}} - v\Delta t; v) + \left( \begin{array}{c} 0 \\ 0 \end{array} \right) g_i(x_{i+\frac{1}{2}}, -v\Delta t; v) \ dv \ dt
$$
CFL Redux: Flux Formulation

- Flux formula depends only on adjacent cells
- CFL restriction for the transport equation!
- Max particle speed $v_{\text{max}}$, timestep $\Delta t$, min cell size $\Delta x_{\text{min}}$ must satisfy
  \[ \Delta t \, v_{\text{max}} < \Delta x_{\text{min}} \]
Direct Transport Formulation

\[ \Delta x_i U_i(\Delta t) = \Delta x_i U_i(0) \]

\[ + \sum_{j \neq i} \int_{T_i} \int_{\mathbb{R}} \left( \frac{1}{v_x^2} \right) f_j(x - v \Delta t; v) + \begin{pmatrix} 0 \\ 0 \end{pmatrix} g_j(x - v \Delta t; v) \, dv \, dx \]

\[ - \sum_{j \neq i} \int_{T_j} \int_{\mathbb{R}} \left( \frac{1}{v_x^2} \right) f_i(x - v \Delta t; v) + \begin{pmatrix} 0 \\ 0 \end{pmatrix} g_j(x - v \Delta t; v) \, dv \, dx \]

CFL constraint vanishes; unconditionally stable explicit scheme...
\begin{itemize}
  \item Choose domain of dependence $\Delta x$; corresponding $\Delta t$ is \textit{independent} of mesh size.
  \item Must compute transport from source cell $S$ to target $T$ during $\Delta t$; only targets within $\Delta x$ considered, need not be adjacent.
    \[
    \int_{x \in S} \int_{x + v\Delta t \in T} \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f_0(x, v) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} g_0(x, v) dv \, dx.
    \]
  \item Simple structure in $v$-space $\implies$ practical to evaluate
  \item Extends to unsplit higher dimensional scheme.
  \item No degradation of accuracy or extra diffusion near small cells.
\end{itemize}
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
Comparison of boundary and mid-channel solution
Channel Convergence Tests

Measure $L_1$, $L_\infty$ convergence in the domain as a whole, and $L_1$ the cells within $\Delta x$ of the boundary.
Channel Aligned Advection

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

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

where

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

and $\nu$ is the coordinate aligned with the channel; solve to $t = 0.2$. 
Channel Aligned Advection

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<th>$\Delta x$</th>
<th>$|e|_1$</th>
<th>$k(L_1)$</th>
<th>$|e|_{1,\partial}$</th>
<th>$k(L_{1,\partial})$</th>
<th>$|e|_\infty$</th>
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Oblique shock reflection

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