Computer Simulations in Solar Physics

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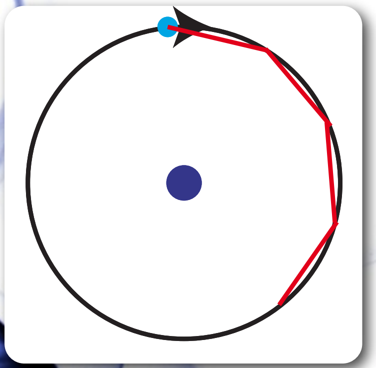
Aims

- Numerical solution of differential equations
  - Techniques
  - Stability
  - Boundary conditions
    - Introduction to parallelism
- Applications to solar physics (MHD)



$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}(\mathbf{v} \wedge \mathbf{B})$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

$$\frac{dv_x}{dt} = \lim_{dt \to 0} \frac{v_x(t + dt) - v_x(t)}{dt}$$

$$\frac{dv_x}{dt} \approx \frac{v_x^{n+1} - v_x^n}{\Delta t}$$

$$\frac{v_x^{n+1} - v_x^n}{\Delta t} = \frac{q}{m}(v_y^n B_z)$$

$$v_x^{n+1} = v_x^n + \frac{\Delta t q}{m}(v_y^n B_z)$$

$$v_y^{n+1} = v_y^n - \frac{\Delta t q}{m}(v_x^n B_z)$$

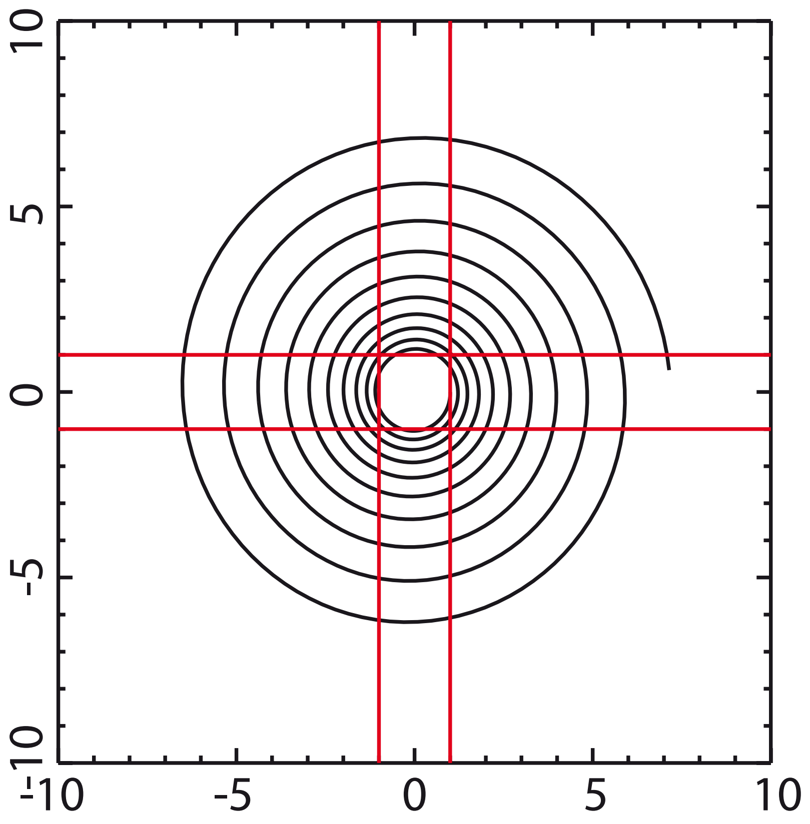
$$x_x^{n+1} = x_x^n + \Delta t v_x^n$$

$$x_y^{n+1} = x_y^n + \Delta t v_y^n$$

$x_x^0 = 0$ $\quad$ $x_y^0 = 1$

$v_x^0 = qBz/m$ $\quad$ $v_y^0 = 0$

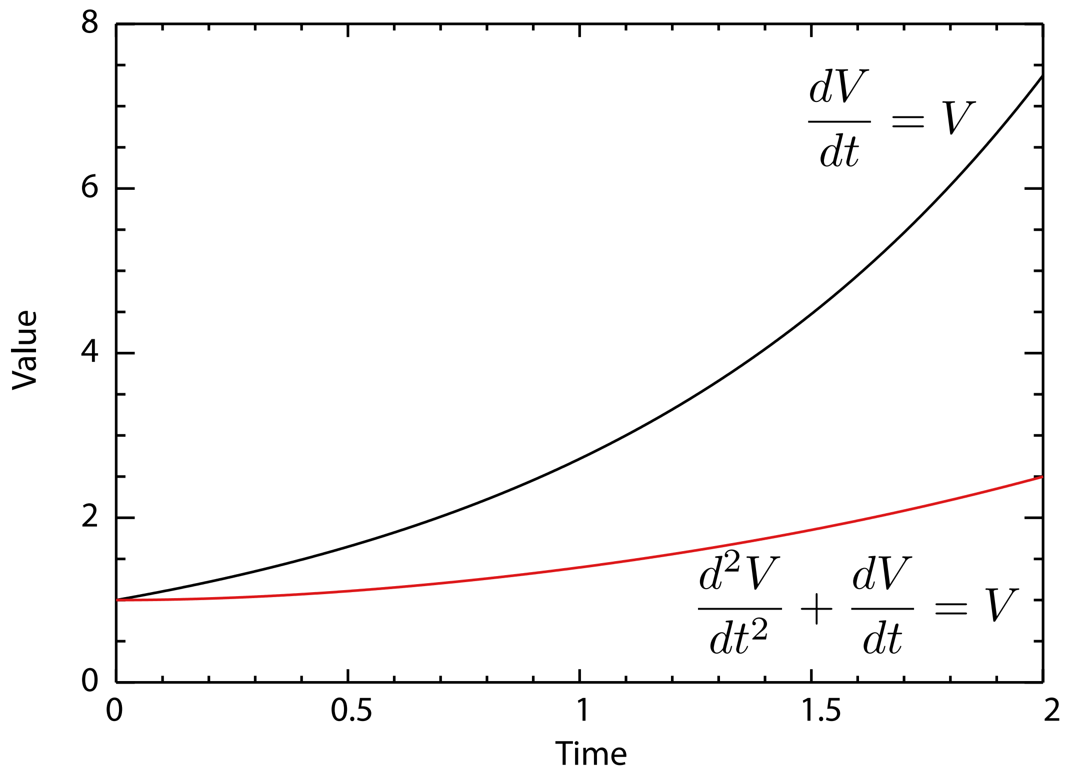
$\Delta t = 0.01\pi m/(qBz)$

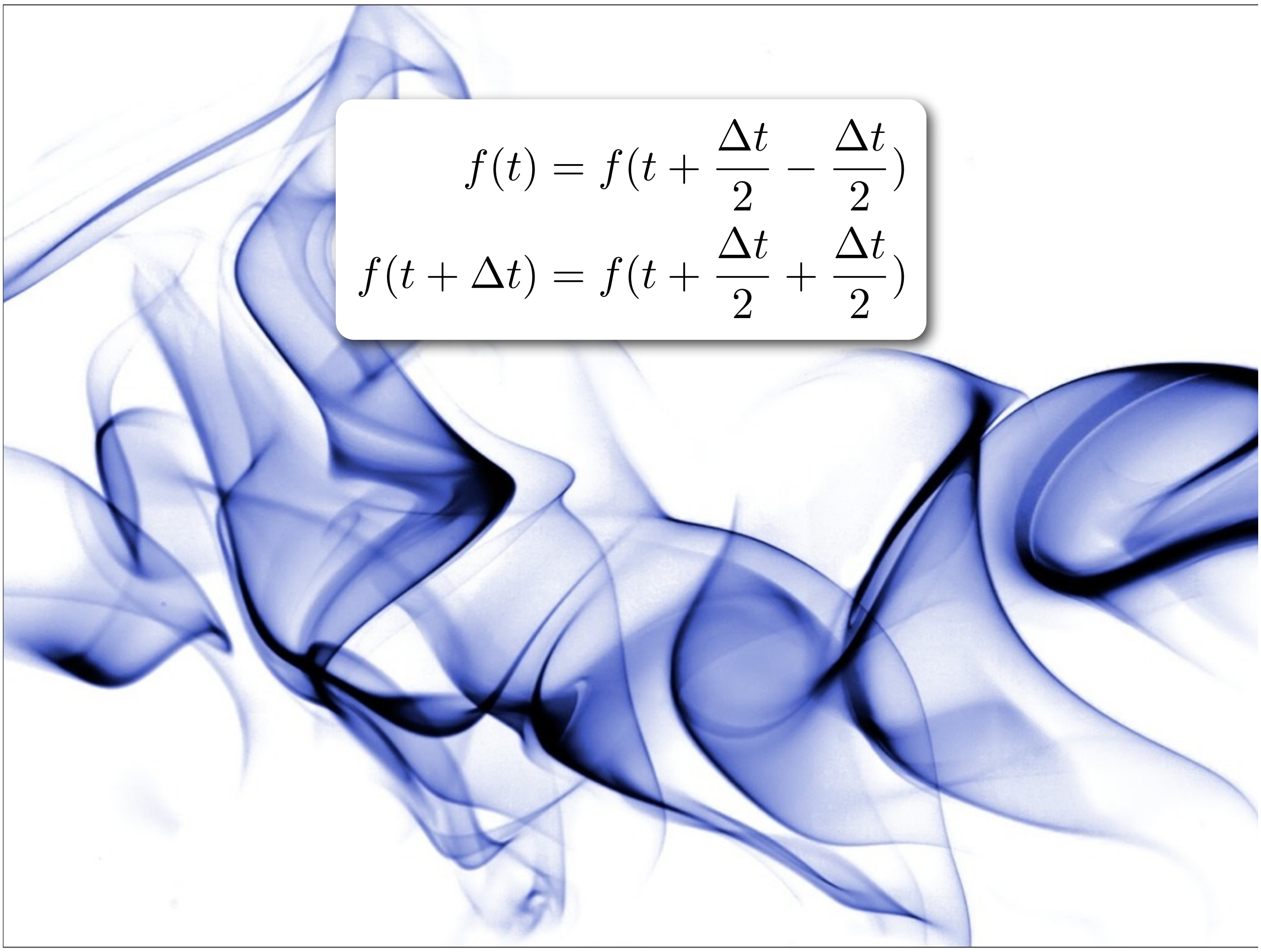


Why didn't it work?

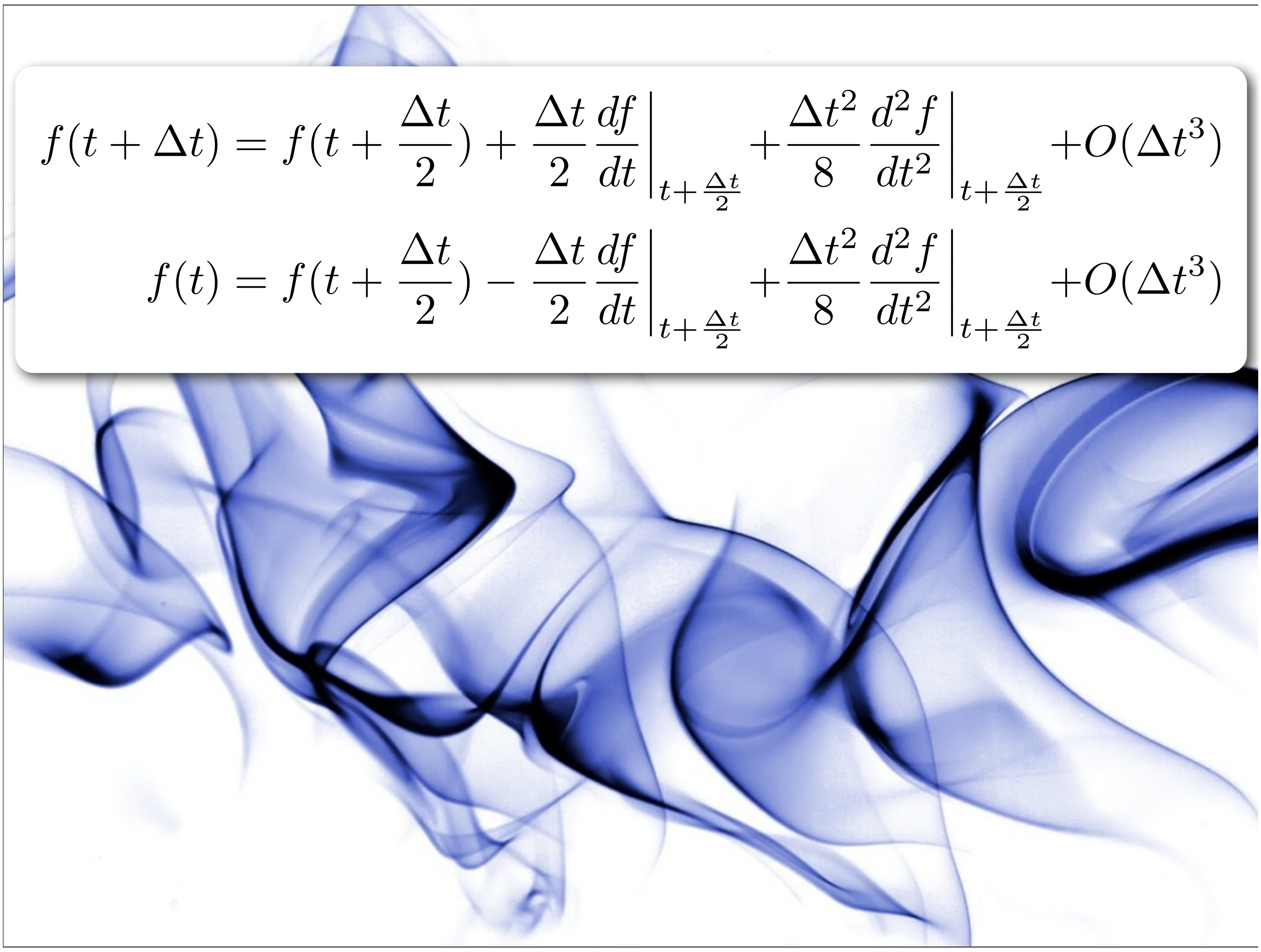
$$f(t+\Delta t) = f(t) + \Delta t \frac{df(t)}{dt}\bigg|_t + \frac{\Delta t^2}{2}\frac{d^2 f(t)}{dt^2}\bigg|_t + O(\Delta t^3)$$

- Ignoring higher order terms
- Effectively diffuses the solution outwards





$$f(t) = f(t + \frac{\Delta t}{2} - \frac{\Delta t}{2})$$
$$f(t + \Delta t) = f(t + \frac{\Delta t}{2} + \frac{\Delta t}{2})$$



$$f(t + \Delta t) = f(t + \frac{\Delta t}{2}) + \frac{\Delta t}{2}\frac{df}{dt}\bigg|_{t+\frac{\Delta t}{2}} + \frac{\Delta t^2}{8}\frac{d^2 f}{dt^2}\bigg|_{t+\frac{\Delta t}{2}} + O(\Delta t^3)$$
$$f(t) = f(t + \frac{\Delta t}{2}) - \frac{\Delta t}{2}\frac{df}{dt}\bigg|_{t+\frac{\Delta t}{2}} + \frac{\Delta t^2}{8}\frac{d^2 f}{dt^2}\bigg|_{t+\frac{\Delta t}{2}} + O(\Delta t^3)$$

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$$f(t) = f(t+\frac{\Delta t}{2}) - \frac{\Delta t}{2}\frac{df}{dt}\bigg|_{t+\frac{\Delta t}{2}} + \frac{\Delta t^2}{8}\frac{d^2 f}{dt^2}\bigg|_{t+\frac{\Delta t}{2}} + O(\Delta t^3)$$

$$\frac{df}{dt}\bigg|_{t+\Delta t/2} \approx \frac{f(t+\Delta t) - f(t)}{\Delta t}$$

- Need to know RHS of equations at half timestep
- Only need to know them to 1st order

$$v_x^{n+\frac{1}{2}} = v_x^n + \frac{\Delta t q}{2m}(v_y^n B_z)$$

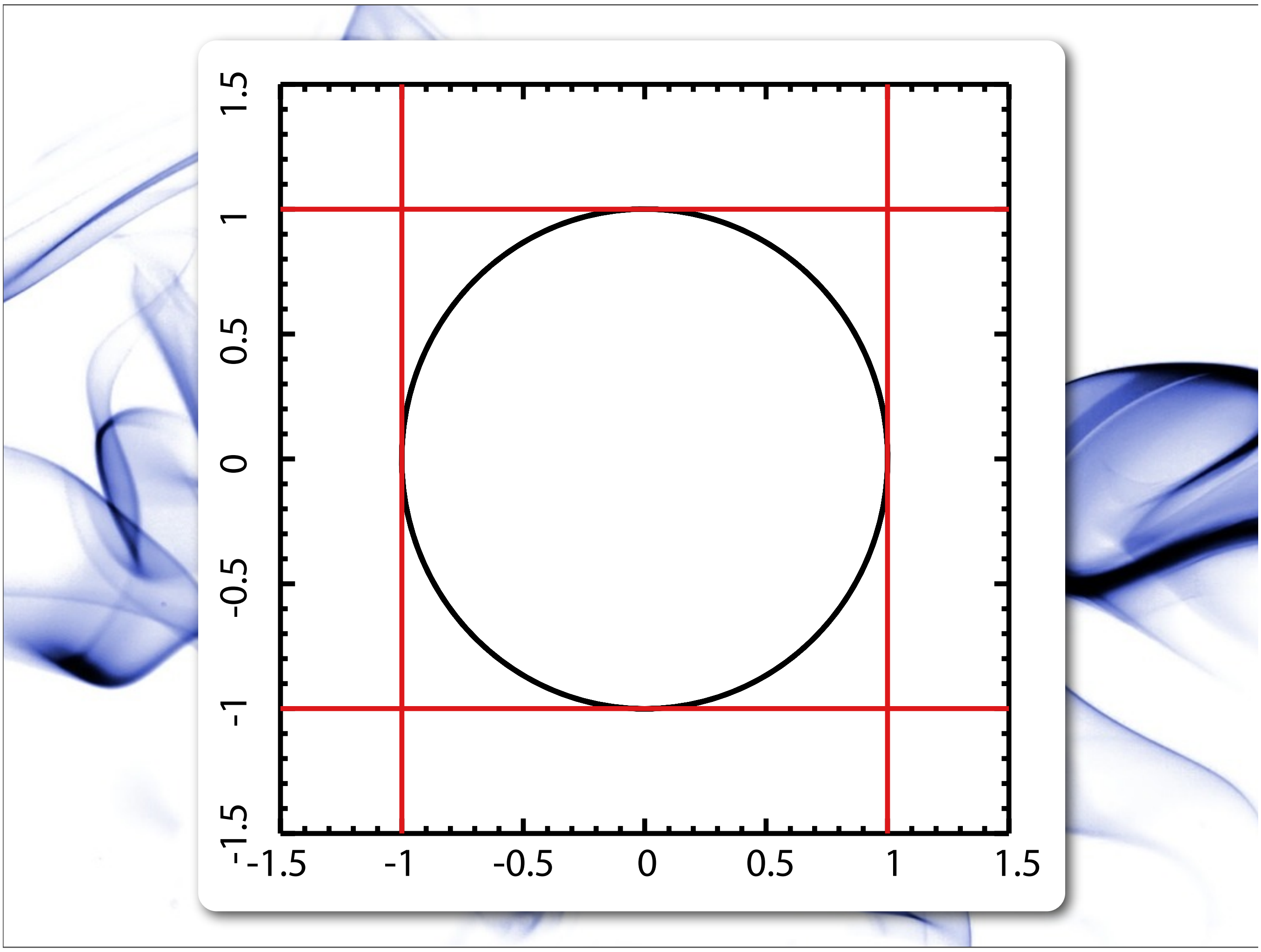
$$v_y^{n+\frac{1}{2}} = v_y^n + \frac{\Delta t q}{2m}(v_x^n B_z)$$

$$x_x^{n+1} = x_x^n + \Delta t v_x^{n+\frac{1}{2}}$$

$$x_y^{n+1} = x_y^n + \Delta t v_y^{n+\frac{1}{2}}$$

$$v_x^{n+1} = v_x^n + \frac{\Delta t q}{m}(v_y^{n+\frac{1}{2}} B_z)$$

$$v_y^{n+1} = v_y^n + \frac{\Delta t q}{m}(v_x^{n+\frac{1}{2}} B_z)$$



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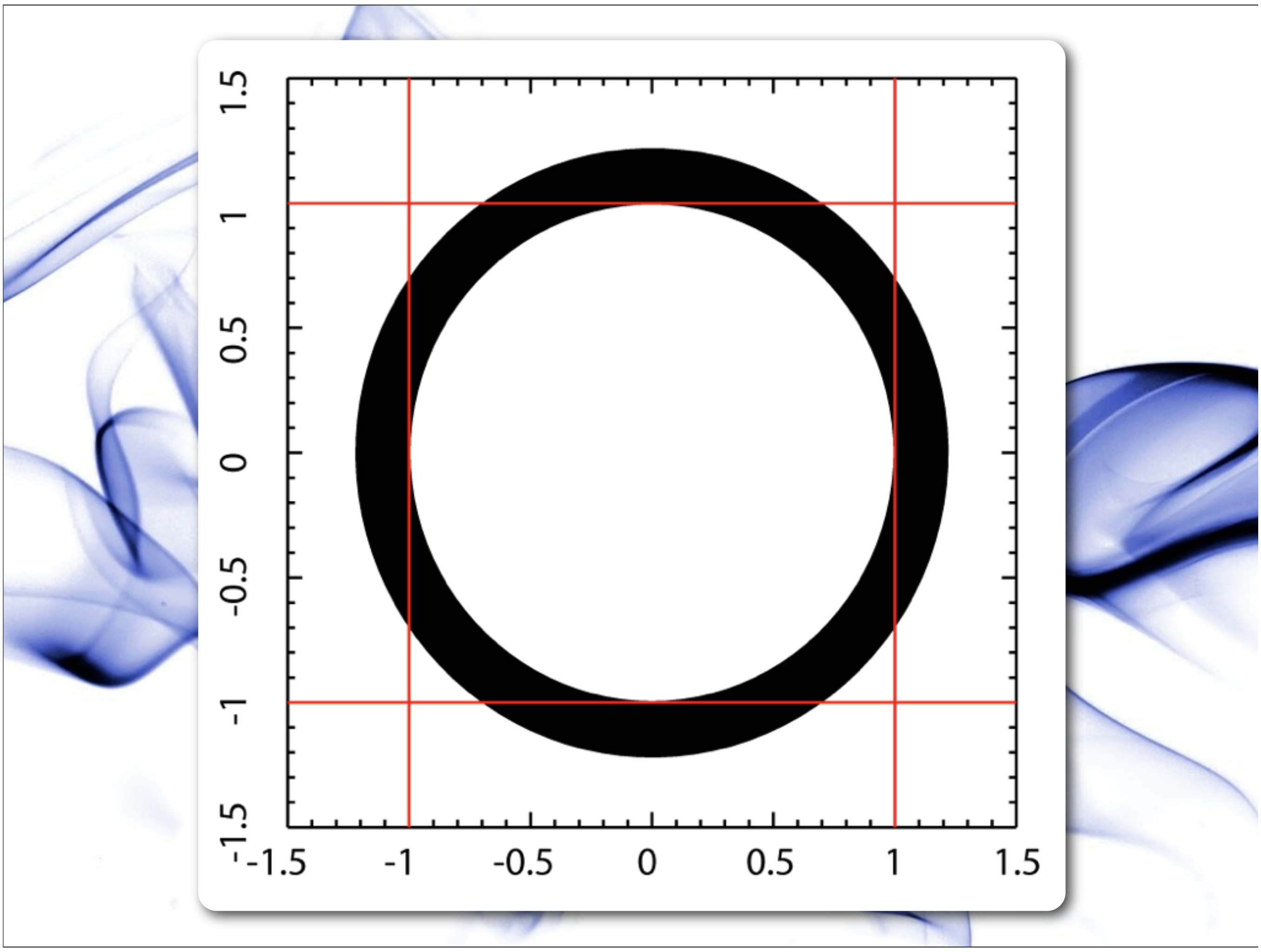

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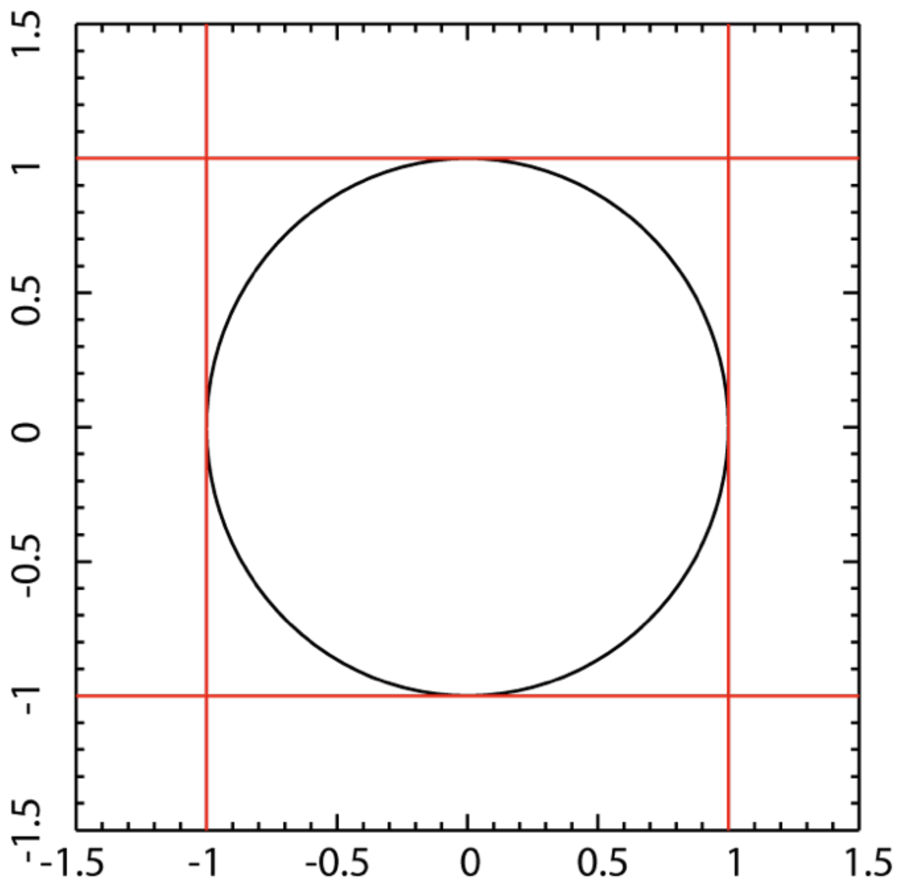
Can we do better?

- Yes. Arbitrarily high order is possible.
- Most common high order time integrator is called the Runge-Kutta 4th order algorithm

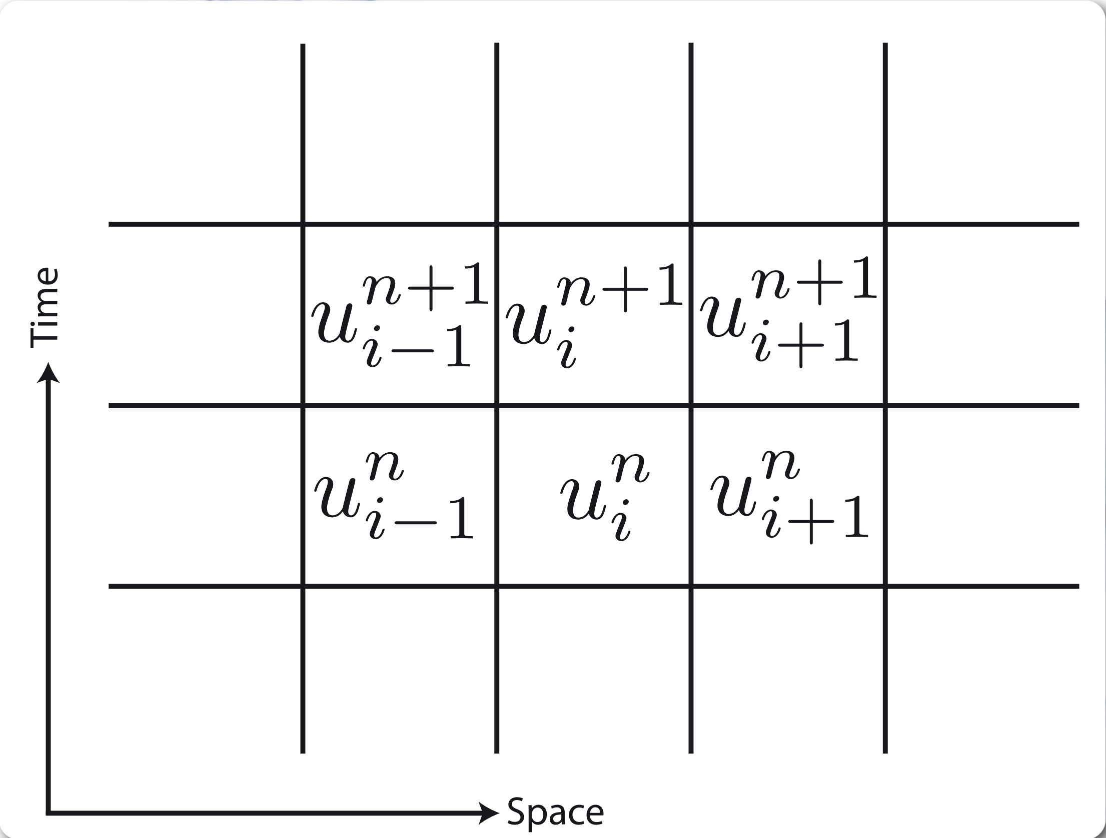
$$
\begin{aligned}
\frac{df(t)}{dt} &= g(f(t), t) \\
k_1 &= \Delta t g(f(t), t) \\
k_2 &= \Delta t g(f(t) + \frac{\Delta t}{2} k_1, t + \frac{\Delta t}{2}) \\
k_3 &= \Delta t g(f(t) + \frac{\Delta t}{2} k_2, t + \frac{\Delta t}{2}) \\
k_4 &= \Delta t g(f(t) + \Delta t k_3, t + \Delta t) \\
f(t + \Delta t) &= f(t) + \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}
\end{aligned}
$$



Conclusions

- Have to have high enough order for problem under consideration
- 4th order good enough for most problems
  - Can use *sympletic* integrator in extreme cases
- For many particles usually use *Boris integrator* instead

Hyperbolic equations



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

$$u(x+\Delta x) = u(x) + \Delta x \left.\frac{\partial u}{\partial x}\right|_x + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_x + O(\Delta x^3)$$

$$u(x-\Delta x) = u(x) - \Delta x \left.\frac{\partial u}{\partial x}\right|_x + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_x + O(\Delta x^3)$$

$$\left.\frac{\partial u}{\partial x}\right|_x = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} + O(\Delta x^3) \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Error terms

- Once again ignoring higher order terms
- Even derivative terms are diffusive
  - Numerical diffusion - energy in wrong place
- Odd derivative terms are dispersive
  - Numerical dispersion - get wave speeds wrong

$$u_i^{n+1} = u_i^n + c\Delta t\left(\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}\right)$$

$$x = [0, L_x]$$

$$\Delta x = L_x / n_x$$

$$u_i^0 = e^{-\left(\frac{x_i - L_x/2}{\sigma}\right)^2}$$

$$\Delta t = \frac{\Delta x}{c}$$

$$u_{n_x+1}^n = u_1^n$$
$$u_0^n = u_{n_x}^n$$

Von Neumann Stability Analysis

- Write the numerical solution as an exact solution S and error terms ε
- Write new equation for the errors and identify how error terms grow from iteration to iteration

$$u_i^n = S_i^n + \epsilon_i^n$$

$$\epsilon_i^{n+1} = S_i^n + \frac{c\Delta t}{2\Delta x}(S_{i+1}^n - S_{i-1}^n) - S_i^{n+1} + \epsilon_i^n + \frac{c\Delta t}{2\Delta x}(\epsilon_{i+1}^n - \epsilon_{i-1}^n)$$

=0 since exact solution

$$\epsilon_i^{n+1} = \epsilon_i^n + \frac{c\Delta t}{2\Delta x}(\epsilon_{i+1}^n - \epsilon_{i-1}^n)$$

$$\epsilon_i^n = \sum_0^{n_x/2} e^{at} e^{ikx}$$

$$\begin{aligned}
\epsilon_i^n &= e^{at} e^{ikx} \\
\epsilon_{i+1}^n &= e^{at} e^{ik(x+\Delta x)} = \epsilon_i^n e^{ik\Delta x} \\
\epsilon_{i-1}^n &= e^{at} e^{ik(x-\Delta x)} = \epsilon_i^n e^{-ik\Delta x}
\end{aligned}$$

$$G = \frac{\epsilon_i^{n+1}}{\epsilon_i^n} = 1 + \frac{c\Delta t}{\Delta x} i \sin(k\Delta x)$$

$$|G| = GG^* = \sqrt{1 + \left(\frac{c\Delta t}{\Delta x}\sin(k\Delta x)\right)^2}$$

- The amplification factor |G| is *always* larger than one
- The error will grow without bounds
- This method is *unconditionally unstable*
- Some methods are *conditionally stable*. There exist values of Δt and Δx that make the scheme stable

Stability of advection schemes

- In fact most "centered" finite difference approximations are unconditionally unstable for pure advection (See Baldauf JCP 227 6638).
- Can be stabilized by adding finite diffusion. Higher order schemes need less diffusion to be stable.
- Alternatively use upwind difference

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$

$$u(x+\Delta x) = u(x) + \Delta x \left.\frac{\partial u}{\partial x}\right|_x + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_x + O(\Delta x^3)$$

$$u(x-\Delta x) = u(x) - \Delta x \left.\frac{\partial u}{\partial x}\right|_x + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_x + O(\Delta x^3)$$

$$\left.\frac{\partial^2 u}{\partial t^2}\right|_x = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^3)$$

$$u_i^{n+1} = u_i^n + \frac{c\Delta t}{2\Delta x}(u_{i+1}^n - u_{i-1}^n) - \frac{\nu\Delta t}{\Delta x^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

$$G = 1 + \frac{c\Delta t}{2\Delta x}(e^{ik\Delta x} - e^{-ik\Delta x}) - \frac{\nu\Delta t}{\Delta x^2}(e^{ik\Delta x} - 2 + e^{-ik\Delta x})$$

$$|G| = \sqrt{\left(1 - 2\frac{\nu\Delta t}{\Delta x^2}(1 - \cos(k\Delta x))\right)^2 + \left(\frac{c\Delta t}{\Delta x}\sin(k\Delta x)\right)^2}$$

$$\frac{\nu \Delta t}{\Delta x^2} \leq \frac{1}{2}$$

$$\frac{c\Delta x}{\nu} = R_c \leq 2$$

$$u_i^{n+1} = u_i^n + c\Delta t\left(\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x}\right)$$

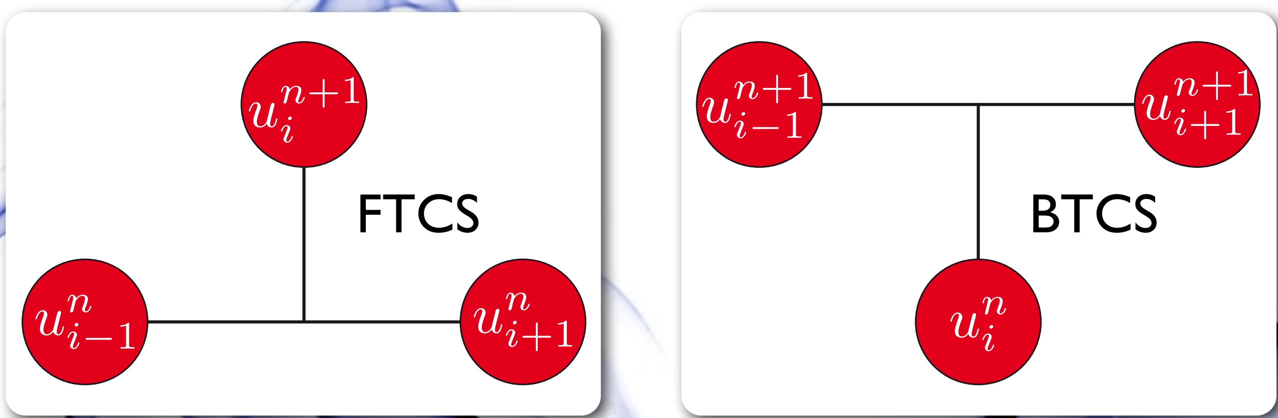
$$|G| = \frac{1}{1 + \left(\frac{c\Delta t}{\Delta x}\right)^2 \sin^2(kx)}$$

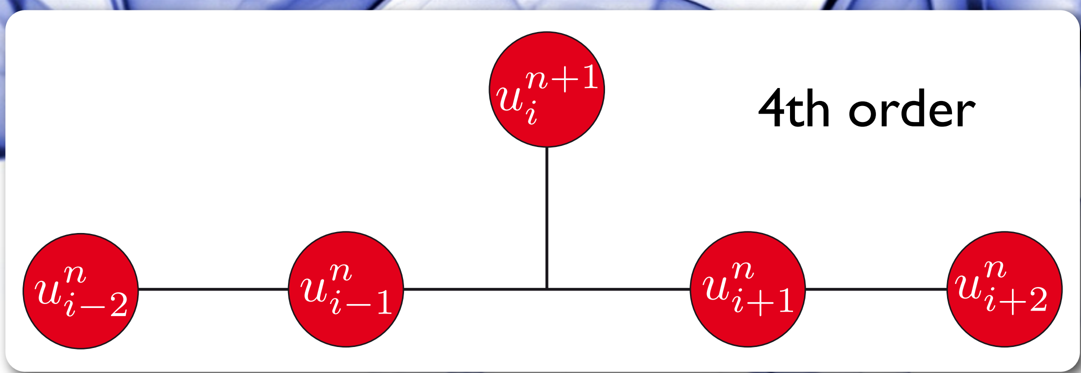
$$\begin{bmatrix} 1 & -a & 0 & 0 & \dots \\ a & 1 & -a & 0 & \dots \\ 0 & a & 1 & -a & \dots \\ 0 & 0 & a & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} u_0^{n+1} \\ u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} u_0^n \\ u_1^n \\ u_2^n \\ u_3^n \\ \vdots \end{bmatrix}$$

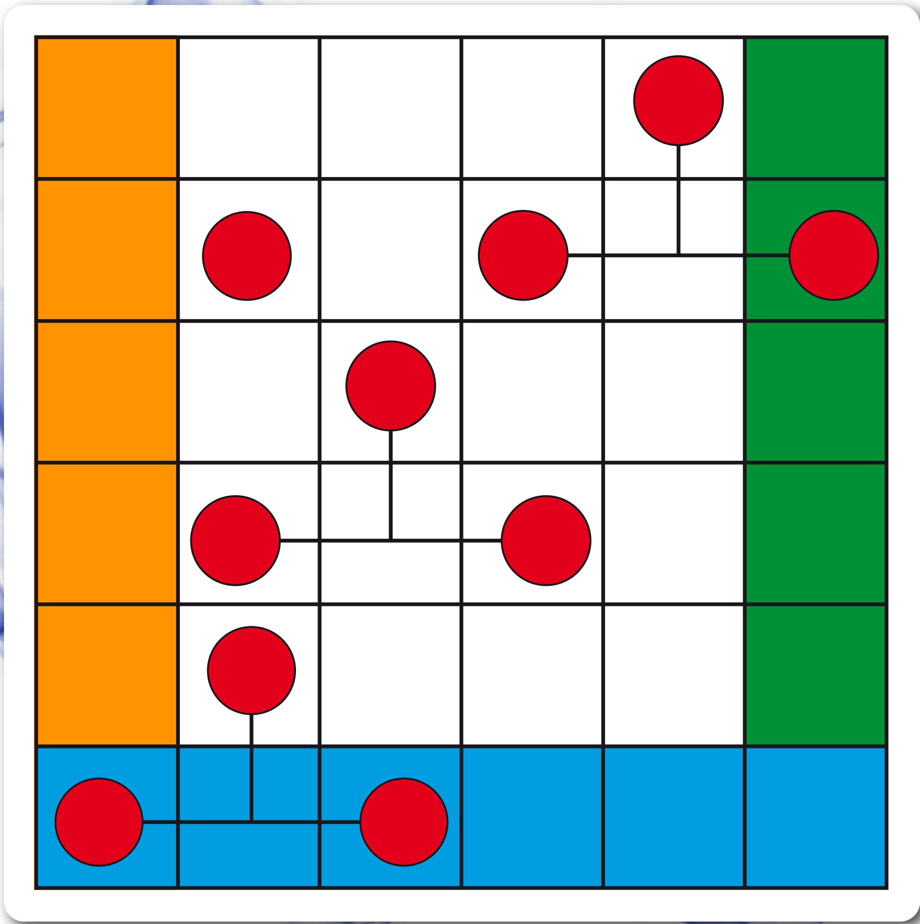
Higher order in space

$$\left.\frac{\partial u}{\partial x}\right|_x^{4th} \approx \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x}$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_x^{4th} \approx \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\Delta x^2}$$







Reflecting boundary

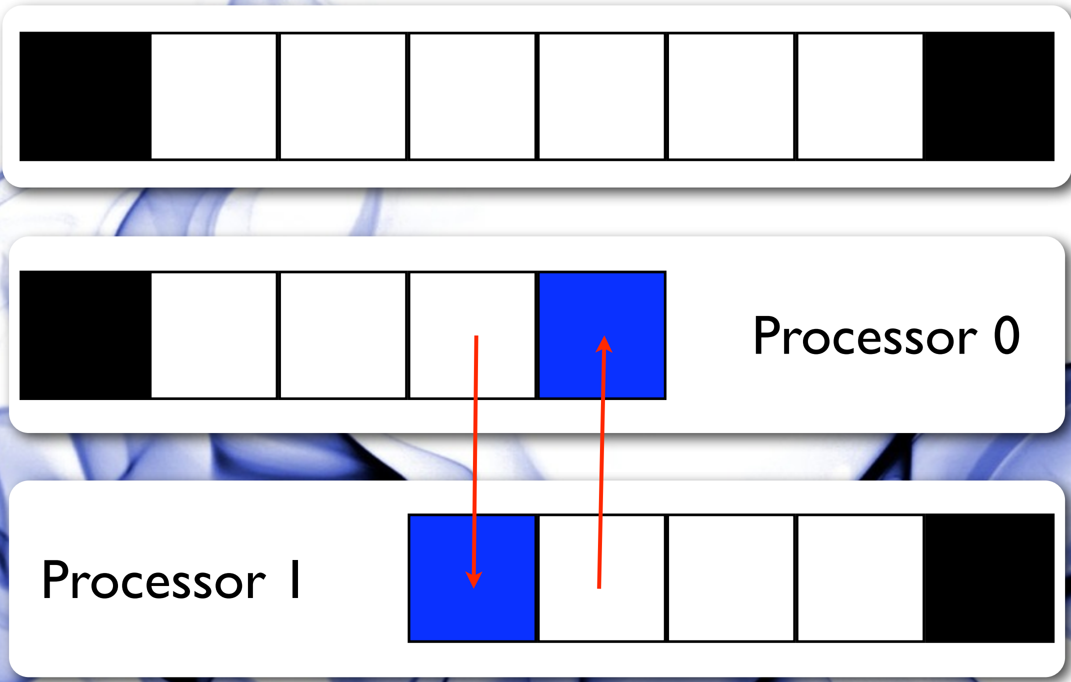
- Can't do for every problem. Not possible for advection equation.
- Needs to be physically correct
  - Density is unchanged at reflecting boundary
  - Velocity reverses sign

Absorbing Boundary

- To do properly need to consider characteristics.
  - Set all outgoing characteristics to still be outgoing
  - Set all incoming characteristics to zero
- Decent first approximation to set the numerical gradient at the boundary to zero

Boundary conditions at high order

- Higher order spatial derivatives have wider stencils
  - Have to specify more ghost cells
  - Essentially specify higher order derivative boundary conditions



- Same principle as boundary conditions
- Copy data from adjacent processor
- Quick and efficient.

Nonlinear equations

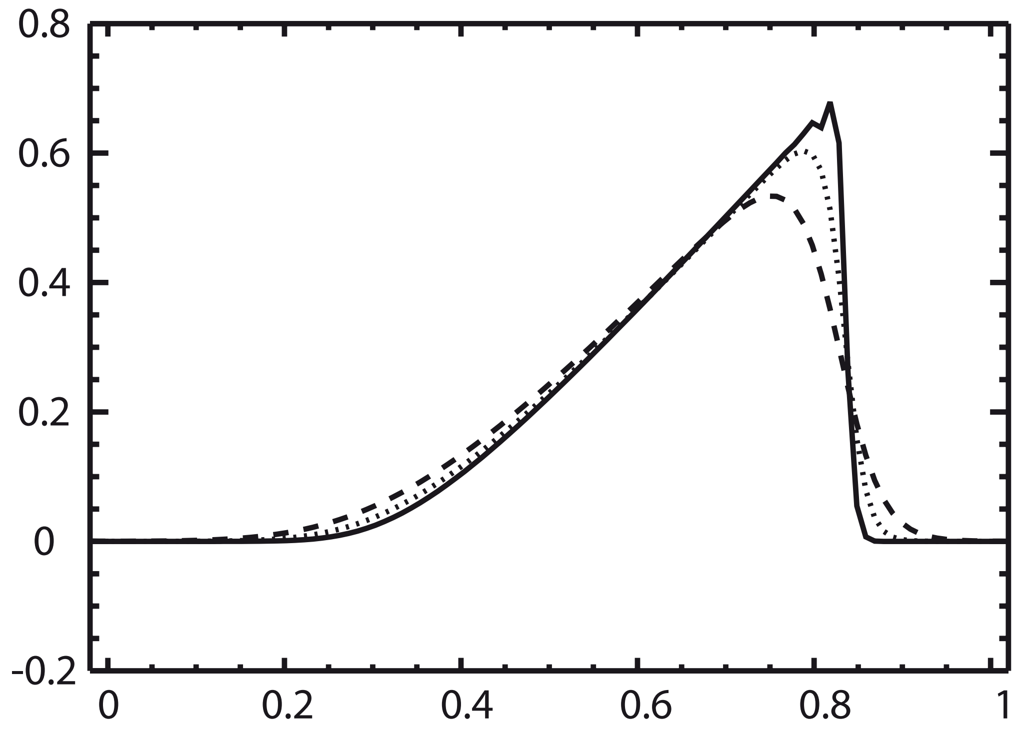
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

$$\Delta t = \frac{\Delta x}{\mathrm{MAXVAL}(u)}$$

- Non-linear problem so can't do von Neumann analysis
- Timestep is created by analogy with the linear advection equation
- Timestep can now change while the code runs

What went wrong now?

- Not the timestep.
- The problem is that the solution steepens into a discontinuity.
  - Differential calculus breaks!
- Odd thing is that we can continue.
  - Viscosity
  - Upwinding



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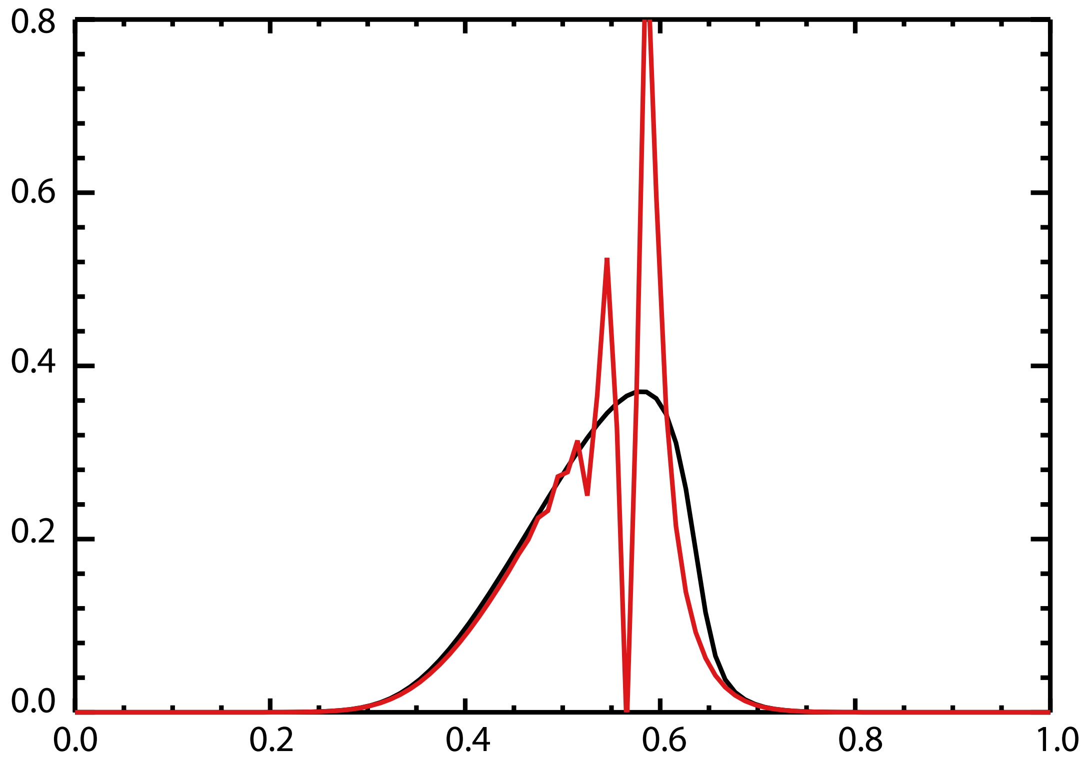
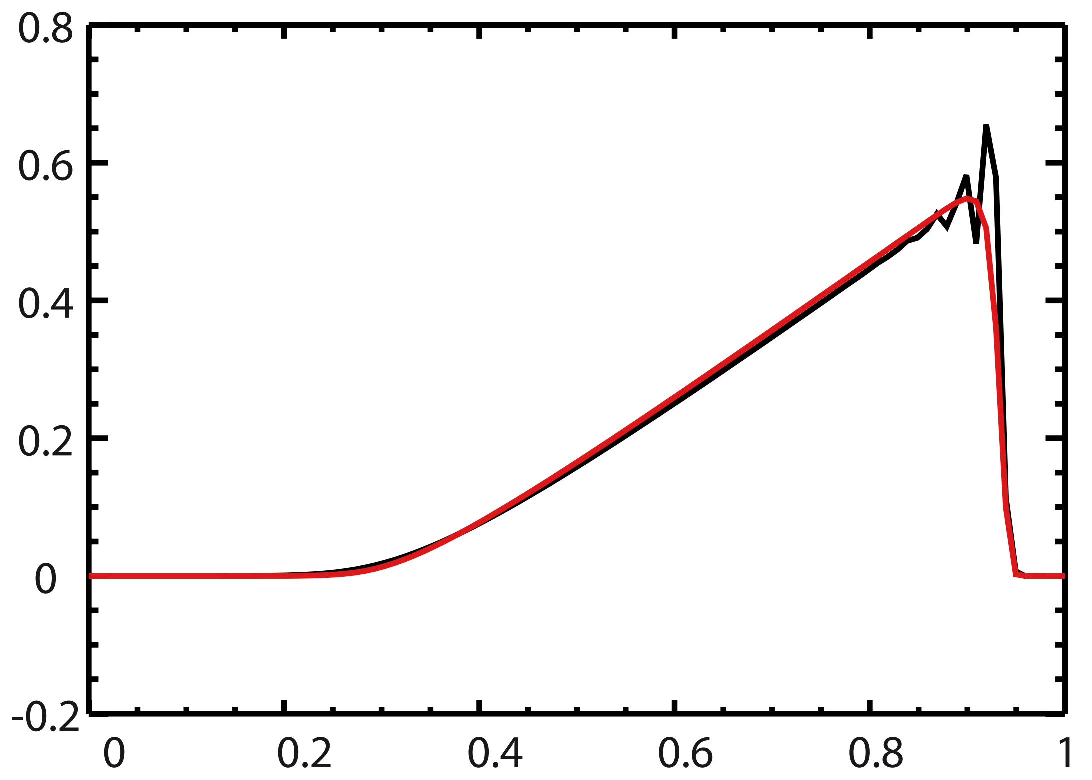
$$\left.\frac{\partial u}{\partial x}\right|_x \approx \frac{u_{i+1} - u_i}{\Delta x}$$

$$\left.\frac{\partial u}{\partial x}\right|_x \approx \frac{u_i - u_{i-1}}{\Delta x}$$

$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0$$





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Upwinding

- Take derivative onesided backwards across shock works!
- Not just diffusion
- Godunov's order barrier theory
  - Only schemes of first order are TVD

$$\left.\frac{\partial u}{\partial x}\right|_x \approx \frac{u_{i+1} - u_i}{\Delta x}$$

Upwind for left traveling objects

$$\left.\frac{\partial u}{\partial x}\right|_x \approx \frac{u_i - u_{i-1}}{\Delta x}$$

Upwind for right traveling objects

Total Variation Diminishing (TVD)

$$TV = \int \left| \frac{\partial u}{\partial x} \right| dx = \sum_i |u_{i+1} - u_i|$$

- TVD is simply that TV decreases every timestep
  - TVD scheme is monotonicity preserving
  - No spurious oscillations

Why not 1st order?

- Leading order error term is second order
  - Large diffusive error
- Works well enough for shocks
- Very poor for smooth solution regions

Hydrodynamics & MHD

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla.(\rho \mathbf{V}) &= 0 \\
\rho \frac{\partial \mathbf{V}}{\partial t} + \rho(\mathbf{V}.\nabla)\mathbf{V} &= \nabla p - \mu^{-1}\mathbf{B} \times \nabla \times \mathbf{B} \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla \times (\mathbf{V} \times \mathbf{B}) \\
\frac{\rho^\gamma}{\gamma - 1} \frac{d}{dt}\left(\frac{p}{\rho^\gamma}\right) &= 0
\end{aligned}
$$

$$p = \frac{\rho T}{\overline{m}}$$

$$\nabla.\mathbf{B} = 0$$

MHD

- Apply techniques above
- Have to find some mechanism to ensure solenoidal condition
  - Flux constrained transport
  - Divergence cleaners

Timestep

$$\begin{aligned}\Delta t &\leq A\frac{\Delta x}{c_f} \\ A &< 1\end{aligned}$$

Finite Difference Code

- Job done
- Good for linear wave problems at high order
- Have to use viscosity to stabilize shocks
- Poor choice for shock dominated problems

Nonlinear Hydrodynamics & MHD

Brief aside

- Viscosity needed to allow finite difference scheme to resolve shock is NOT shock viscosity
- Real shocks have entropy jump across shock
- This corresponds to a real, physical, shock viscosity.

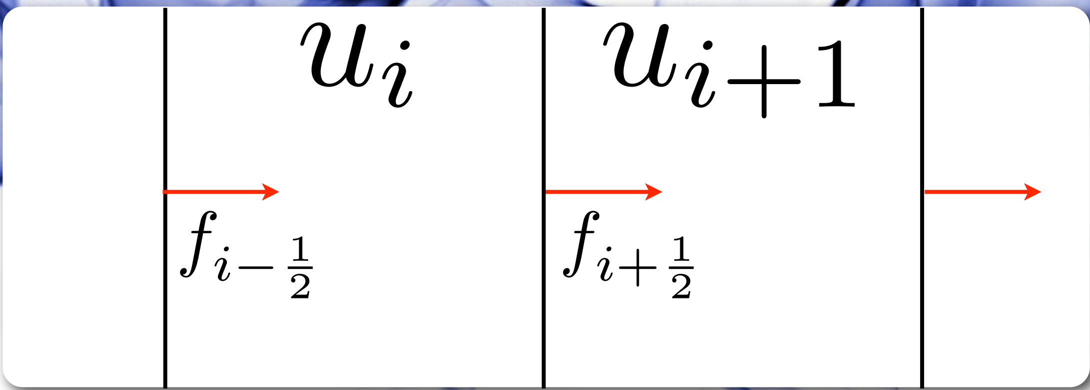
Conservative form

$$\frac{\partial u}{\partial t} + \nabla . f = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial u^2/2}{\partial x} = 0$$

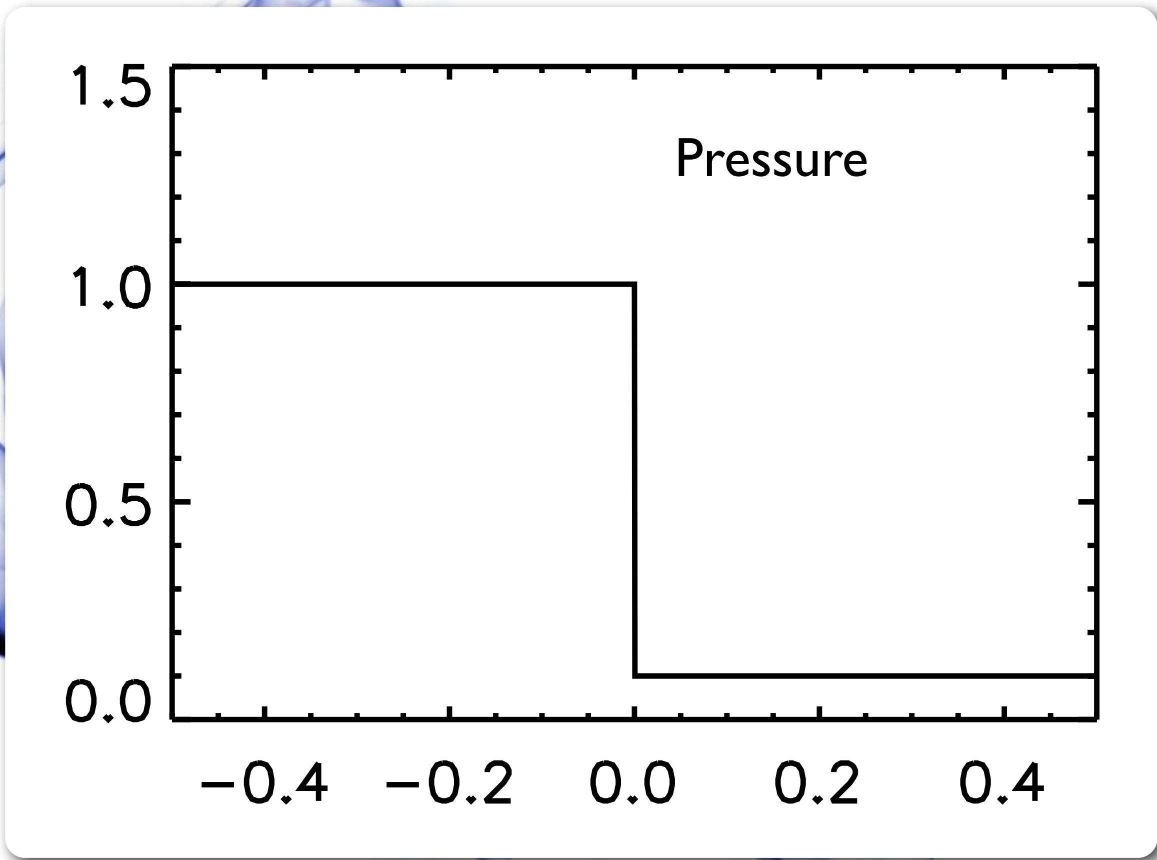
Conservative form

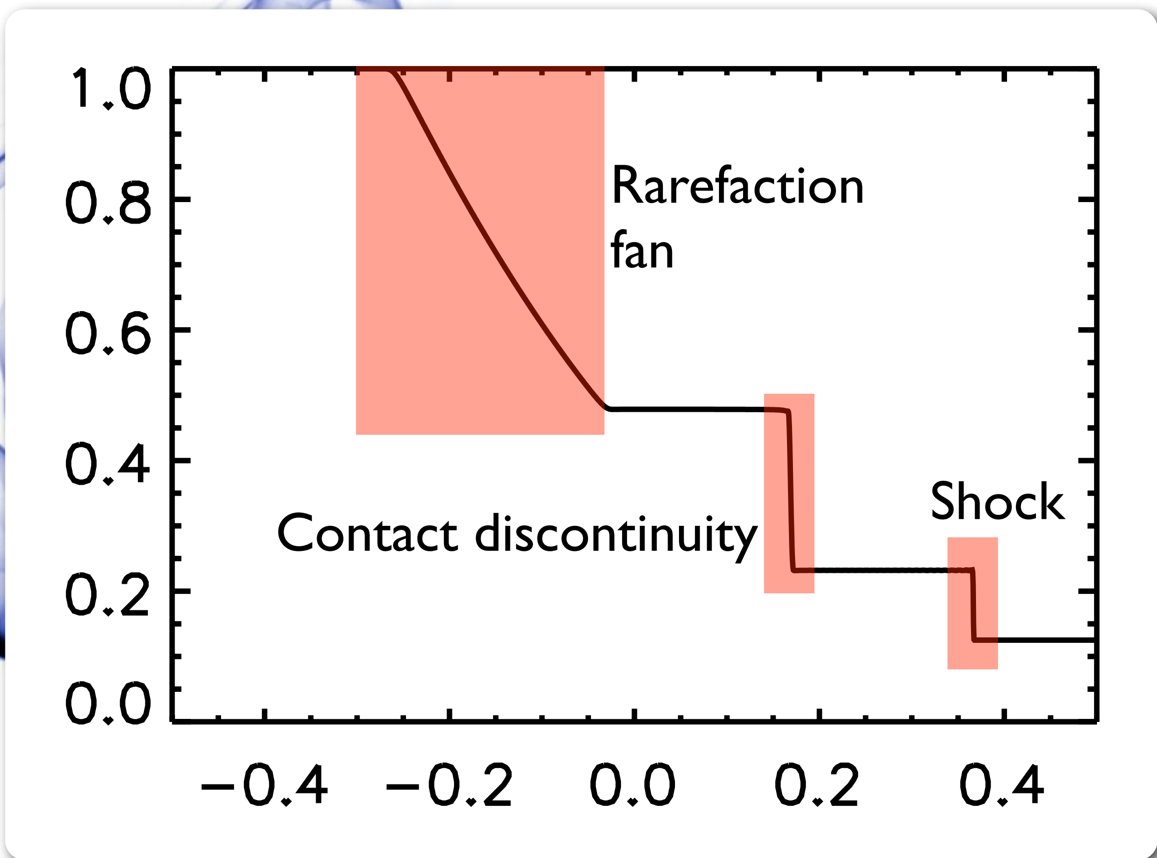
$$u_i^{n+1} = u_i^n + \Delta t(f_{i-\frac{1}{2}} - f_{i+\frac{1}{2}})$$



Choices

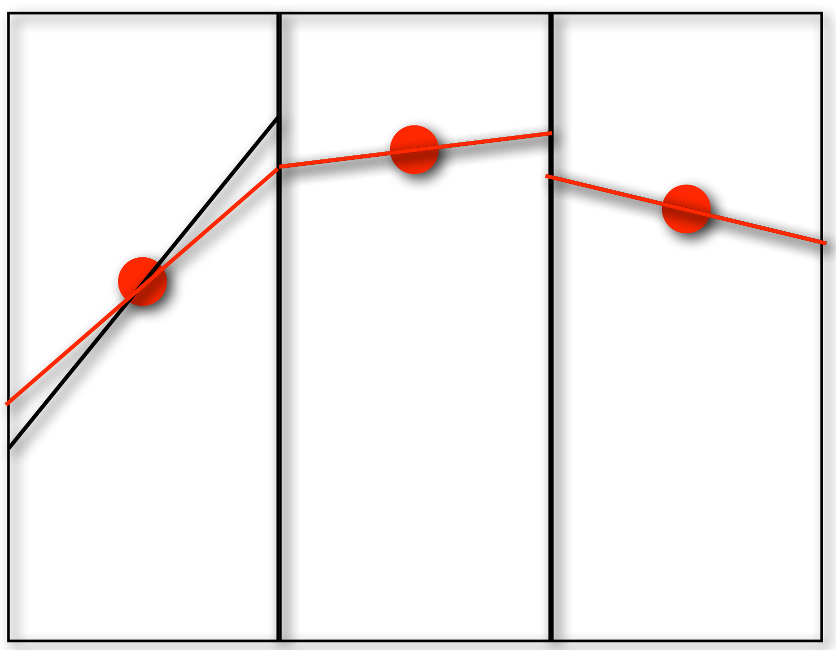
- Say flux at edge is the same as flux in the centre.
  - If always select flux in upwind direction then equivalent to upwinding in finite difference
- Flux limiters - Weighted average of upwind and high order reconstruction
- Godunov schemes - Riemann solvers


Pressure
1.5
1.0
0.5
0.0
−0.4
−0.2
0.0
0.2
0.4

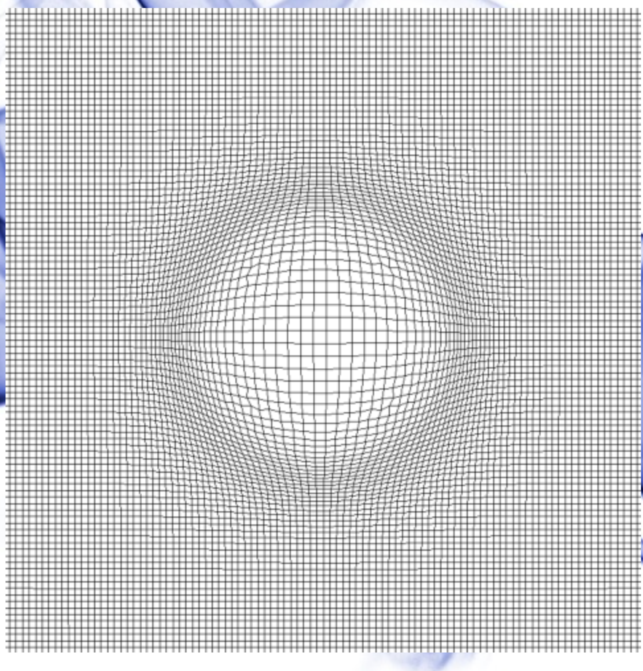

Rarefaction
fan
Contact discontinuity
Shock
1.0
0.8
0.6
0.4
0.2
0.0
−0.4
−0.2
0.0
0.2
0.4

MUSCL Scheme

- Monotone Upwind for Scalar Conservation Law scheme
- Bram van Leer 1979
- Godunov type scheme where states are not assumed to be simple piecewise linear blocks
- Some Riemann-solver less versions



Lagrangian Codes



- Mesh follows fluid flow
- Mesh is compressed at shocks
- Mesh can tangle for rotational flows

Lagrangian Remap

- Take Lagrangian step
- Remap back to original grid
- So long as remap using flux limiters scheme is shock capturing
- Good example is Warwick's own LARE code

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ALE Codes

- Arbitrary Lagrangian Eulerian
- Like Lagrangian Remap, but don't have to remap every step and don't have to remap back to original grid
- Good shock performance, good linear wave performance
- Specialised and hard to program

AMR

- Adaptive mesh refinement
- Locally adjusts the grid spacing in "interesting" regions
- Allows problems to be run on smaller computers
- Only works well for certain problems

Words on developing codes

- Most of the work in developing scientific software is not science related
  - Structure design
  - Parallelism
  - Output and visualisation
  - User interaction