Computational techniques for conservation law PDEs

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Summary

Derivations

- Start with Taylor's series of an arbitrary function

$$f(x+\Delta x) = f(x) + \frac{f'(x)}{1!}\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \frac{f'''(x)}{3!}\Delta x^3 + \dots$$

- Solve for $f'(x)$

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} + \mathcal{O}(\Delta x)$$

- One can approximate by truncating $\mathcal{O}(\Delta x)$

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

- Same idea can be used for higher order derivatives, with some maths tricks

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Example: The 1-D Heat Equation

- Consider the 1-D heat equation

$$\boxed{\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}}$$

- Discretise the equation

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

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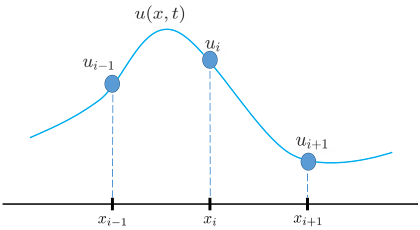
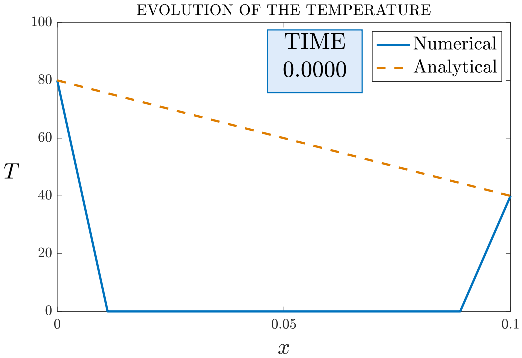


Example: The 1-D Heat Equation (central difference method)

$$\begin{cases} u(0,t) = 80 \\ u(0.1,t) = 40 \\ u(x,0) = 0 \end{cases}$$



Properties of the scheme

Choice of Δt or Δx is limited

For a linear, well-posed PDE, the numerical scheme converges if

1. It is consistent, i.e. $\lim_{\Delta x, \Delta t \to 0}$Truncating Error $= 0$
2. and stable, i.e. $|\frac{u_i^{n+1}}{u_i^n}| \leq 1 \xrightarrow{\text{stability analysis}}$ the CFL condition, usually $\frac{\lambda_{max}\Delta t}{\Delta x} \leq 1$

Explicit and implicit methods

- Explicit method, u_i^{n+1} is obtained directly from $u_{i-1}^n, u_i^n, u_{i+1}^n$
- Implicit method, u_i^{n+1} is expressed in terms of both known and unknown quantities at time n and n+1 and is obtained by solving a system of algebraic equations. It requires more computation power but allows larger Δt

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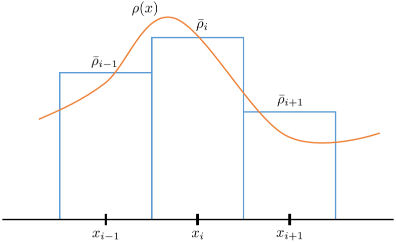
Summary

Derivations

Consider the advection equation

$$\frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = s(x)$$



- Compute the cell averages for all i, defined as

$$\bar{\rho}_i = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x)dx$$

- Reconstruct the values in each cell from cell averages
- Different reconstruction orders are possible: piece-wise constant, linear, quadratic, etc.

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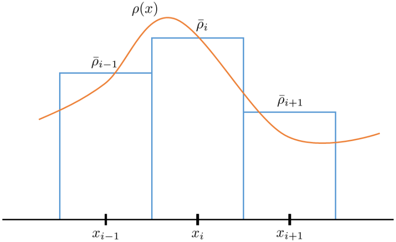

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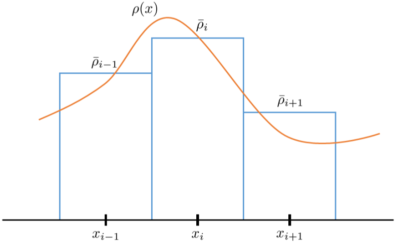

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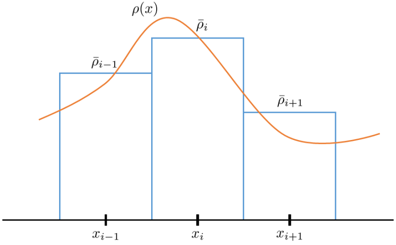

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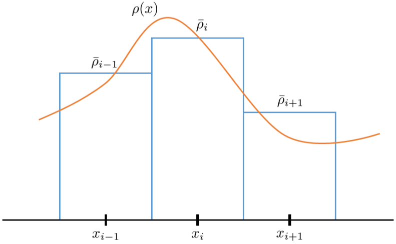

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Derivations

- Consider fluxes at the cell boundaries, i.e. $F_{i-1/2}$, $F_{i+1/2}$, in this case

$$F(\rho) = c\rho$$

- Apply divergence theorem at the boundaries and discretise the equation

$$\frac{\bar{\rho}_i^{n+1} - \bar{\rho}_i^n}{\Delta t} = -\frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x} + s_i^n$$

- Compute the fluxes by numerical flux functions

$$F_{i+1/2}(\rho) = \tilde{F}(\rho_1, \ldots, \rho_i, \rho_{i+1}, \ldots, \rho_n)$$

- At steady state, analytically $\partial_x F = s(x)$

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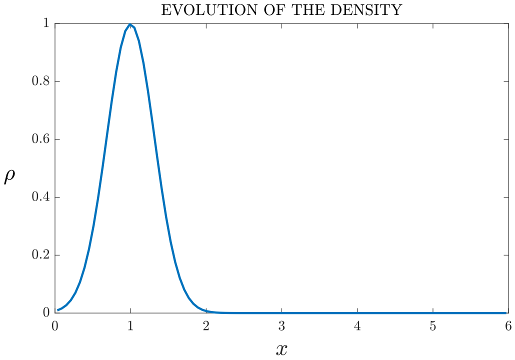
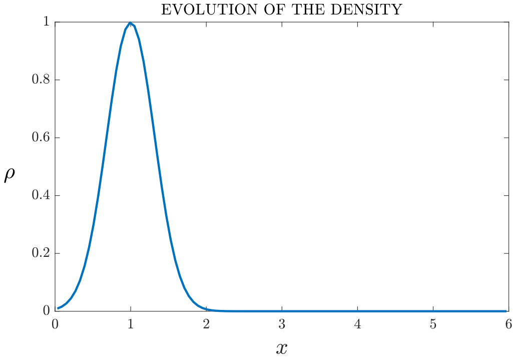
Example 1: The Advection Equation (backward method)

$$\frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = 0$$



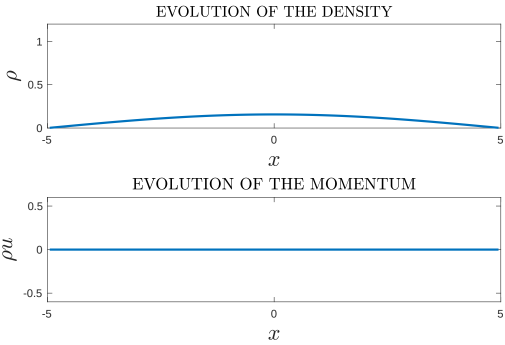
Example 2: The Burgers' Equation (upwind method)

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



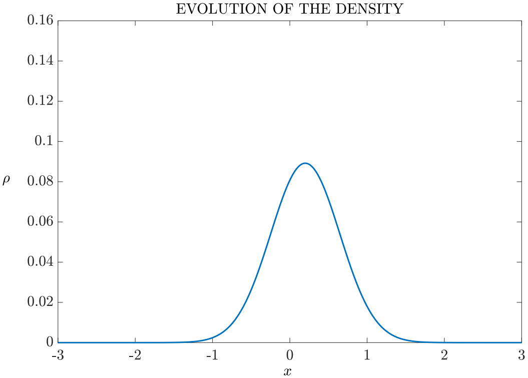
Example 3: The Euler Equations (local Lax-Friedrich method)

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + \rho) = -\rho \partial_x \dfrac{x^2}{2} \end{cases}$$



Example 4: The Gradient Flow Equation (method by Carrillo, Chertock, Huang)

$$\partial_t \rho = \partial_x(\rho \partial_x(\rho + \frac{x^4}{4} - \frac{x^2}{2}))$$



Summary

The Hard Sphere Model

Hard spheres are model particles used widely in the statistical mechanics of fluids and solids

They cannot overlap and are defined in terms of potentials

$$V(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} 0 & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| \geq \sigma \\ \infty & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| < \sigma \end{cases}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of particles and σ is the diameter of particles

The objective is to investigate the evolution of density of the hard spheres in a 1-D box under an external potential

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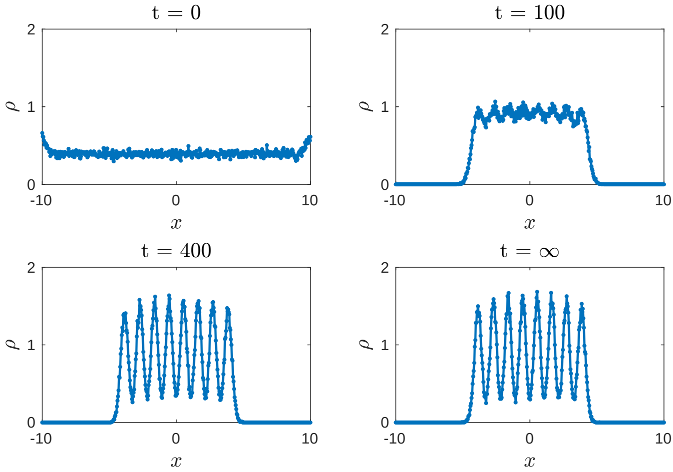
The Metropolis Monte Carlo algorithm

Steps in the algorithm

1. Set an initial configuration C_i, where i $= 0$
2. Randomly generate a new state C_j from the current configuration
3. Compute the potential change between the two states, i.e. $U_j - U_i$
4. Accept the new state with a probability of $exp(-(U_j - U_i))$
5. Increase i by 1 and return to step 2

MC simulation of hard spheres in a 1-D box under an external potential of x^2



Summary

Unlike in Monte Carlo where a fixed recipe is conceived for the particles to generate new states, in MD the new states are determined by the integration of Newton's equations of motion

For instance, the Velocity Verlet method

$$\begin{cases} \vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \dfrac{\vec{F}(t)}{2m}\Delta t^2 \\ \vec{v}(t+\Delta t) = \vec{v}(t) + \dfrac{\vec{F}(t)+\vec{F}(t+\Delta t)}{2m}\Delta t \end{cases}$$

For the same hard sphere model, since $\vec{F}(t) = -\nabla V$, the WCA potential (which is continuous) is used

$$V(r) = 4[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}] \quad \text{for} \quad r < 2^{1/6}\sigma$$

where r is the distance between particles and σ is the diameter of particles

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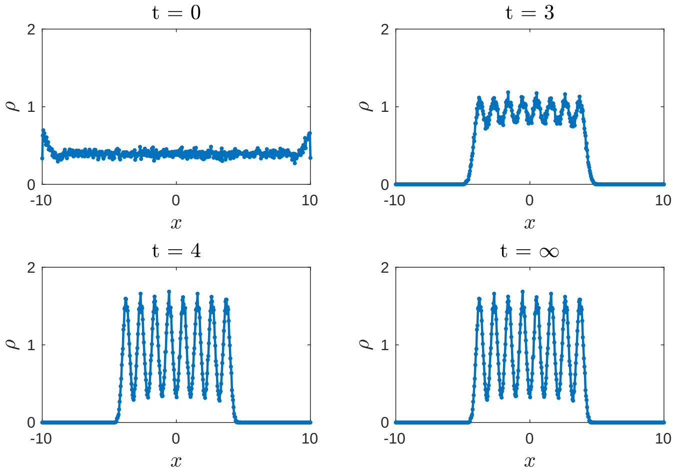

Comparison between MC and MD