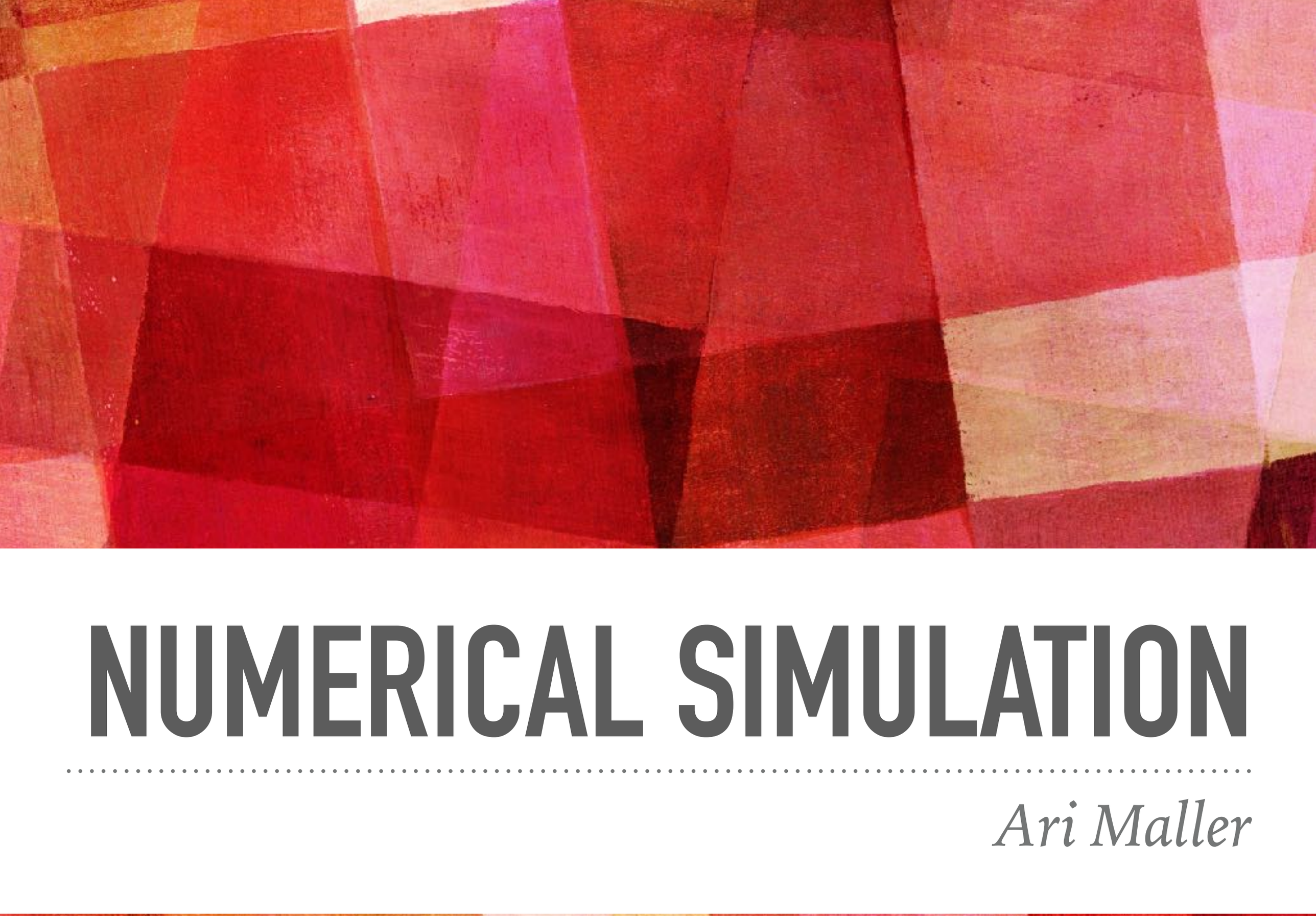


NUMERICAL SIMULATION

Ari Maller

NUMERICAL SIMULATION

- One of the main uses of computers in the sciences is for performing numerical simulations.
- The use of the term simulation can be confusing because it is often used interchangeably with modeling. One might say they have made a simulation of a phenomena, meaning they have made a model of the phenomena.
- I will try to use numerical simulation to mean a numerical technique where a phenomena is modeled by having elements of it represented in a computer and then evolved following certain rules.
- Those rules can ODEs or PDEs or logic or anything else. The key aspect of a numerical simulation is that one does not know the future state of the system on which the rules will be applied.

soccer example - https://www.youtube.com/watch?v=cP035M_w82s

WHAT IS AN ELEMENT?

- In some situations what should be an element in the simulation is obvious. For example simulating the motion of the planets each planet should be an element.
- However, if you also want to simulate the stresses on the planets by tidal forces, or the possible destruction of a moon, then treating the planets as point particles won't work.
- Instead you might have to have each element in the simulation be a piece of a planet, so that a planet would be made up of hundreds or thousands of pieces.
- Thinking about what the elements are in a simulation, what limitations that imposes and how the simulation would be different with different elements is an important aspect of numerical simulation.

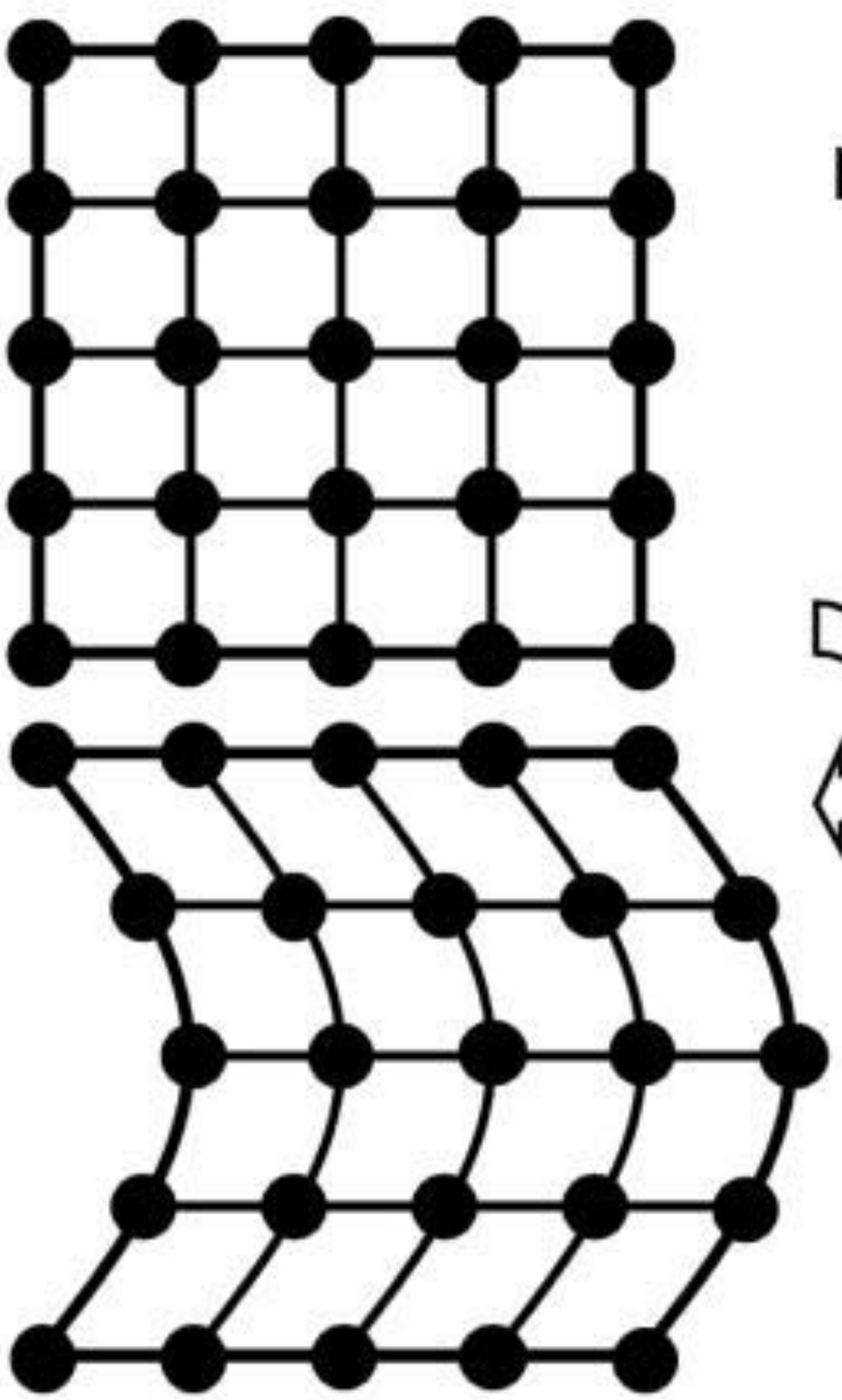
FLUID MECHANICS

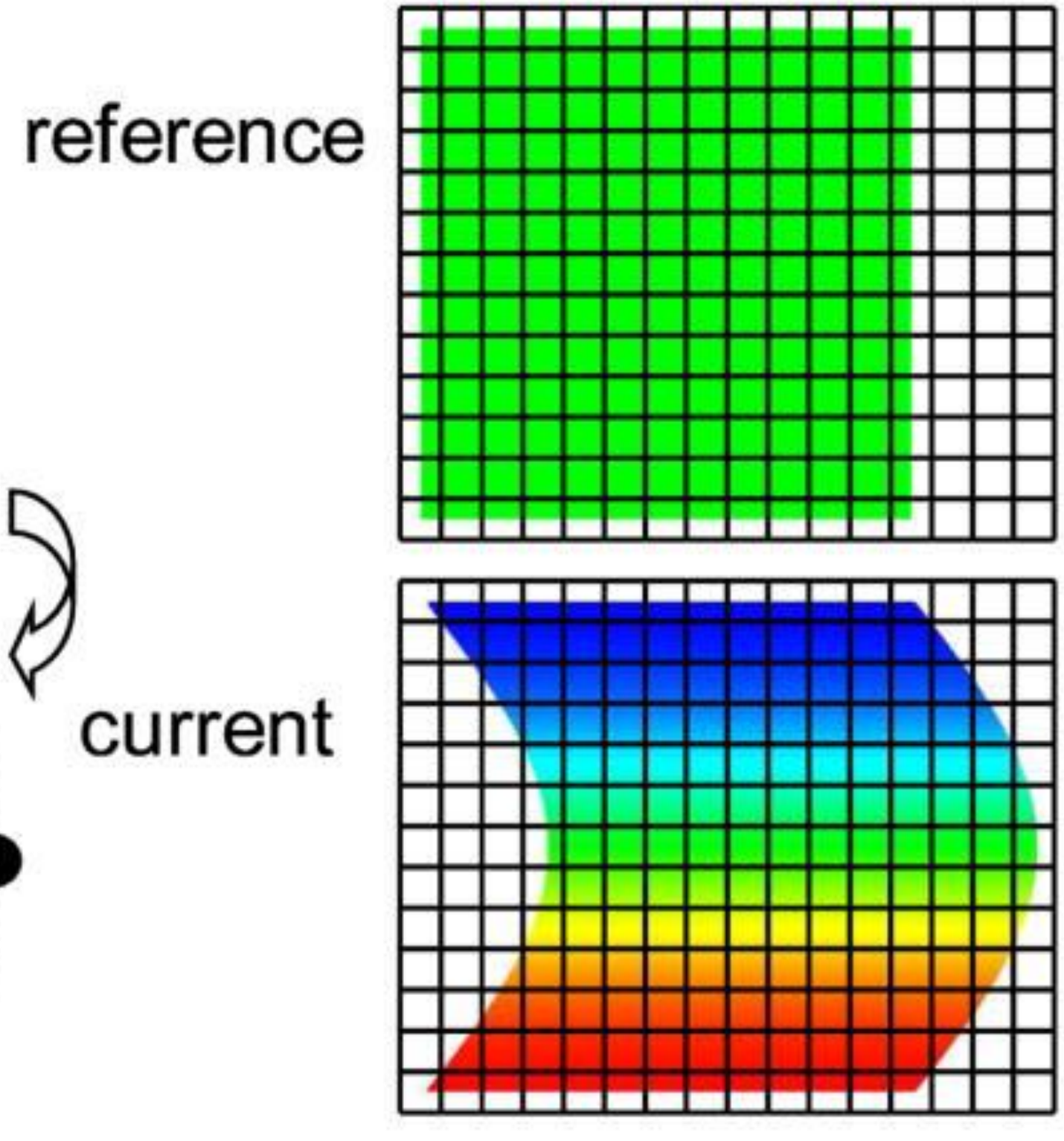
- One area of physics where numerical simulation plays an enormous role is fluid mechanics. This is largely because almost all fluid mechanics problems are unsolvable analytically.
- In fluid mechanics a fluid has some properties that can have differing values as every point in space and can change with time.
- A simple set up can lead to a wide range of behaviors like the Kelvin-Helmholtz instability you see here.

video - https://www.youtube.com/watch?v=qEGbzZM0Baw

HOW TO WE REPRESENT OUR FIELD

- One interesting thing about fluid mechanics is that there are a number of ways of representing the fluid in space and thus implementing a simulation of the fluid.
- One way to picture a fluid is to make a grid of space and then to view the fluid as flowing through the grid. This is called the Eulerian approach. In it the fluid has certain properties in each cell, and then those properties change as new fluid flows in and out of the cell boundaries.
- An alternative picture is to picture a mass element of the fluid and then let it move along as the fluid flows. This is called the Lagrangian approach. In it each element reacts to the hydro dynamical forces changing its position, density and temperature.





(a) Lagrangian approach

(b) Present Eulerian approach

EQUATIONS OF FLUID DYNAMICS

- The equations of fluid dynamics are based on the three main conservation laws; conservation of mass, conservation of momentum (or Newton's Second Law), and conservation of energy (or the First Law of Thermodynamics).
- This conservation laws can be expressed in integral or differential form, we will focus on the differential form.
- Conservation of mass, or the continuity equation can be written for a fluid with density ρ and flow velocity $\mathbf{u}$ as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

- If we think of the fluid in a cell, then this says the change of density in the cell is given by the rate at which the fluid flows into or out of the cell.

MATERIAL DERIVATIVE

- We have discussed how there are different ways to view fluid flow, the Lagrangian and Eulerian approaches. These difference were not developed for simulations, but for the calculus of the equations. If our coordinates are going to flow with the fluid then

$$\frac{d}{dt}\phi(\mathbf{x},t) = \frac{\partial\phi}{\partial t} + \dot{\mathbf{x}}\cdot\nabla\phi$$

- We can define dx/dt = u the flow of the fluid and then a material or convective or Lagrangian derivative as

$$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi$$

- When expressed in Lagrangian form fluid equations are expressed using this derivative.

CONSERVATION OF MOMENTUM

- The general, non-relativistic form of momentum conservation is given by the Cauchy momentum equation. In Lagrangian (convective) form it is

$$\frac{D\mathbf{u}}{Dt} = \frac{1}{\rho}\nabla \cdot \sigma + \mathbf{g}$$

- where $\boldsymbol{\sigma}$ is the stress tensor and $\mathbf{g}$ represents all *body* forces like gravity, electricity-magnetism, etc.
- In Eulerian (conservative) form the equation becomes

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla \cdot (\rho\mathbf{u}\mathbf{u}^T) = -\nabla \cdot P\mathbf{I} + \nabla \cdot \tau + \rho\mathbf{g}$$

- The left hand side is just converting the material derivative while the right hand side we have also broken the stress tensor into the diagonal terms (pressure) and off diagonal elements.

NAVIER-STOKES EQUATION

- This equation is usually simplified by assuming symmetries. If we assume the stress tensor is isotropic and Galileian invariant then the stresses can be expressed as a scalar v which is called the viscosity. Under these assumptions we get the Navier-Stokes equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla P + \nu \nabla^2 \mathbf{u} + \frac{1}{3}\nu \nabla(\nabla \cdot \mathbf{u}) + \rho \mathbf{g}$$

- If the fluid is incompressible, like many liquids, then $\nabla \cdot \mathbf{u} = 0$ and the Navier-Stokes equation reduces to

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla P + \nu \nabla^2 \mathbf{u} + \rho \mathbf{g}$$

EULER'S EQUATIONS

- A further simplification that is applicable in some situations is to ignore the viscosity, v=0. Then we recover a momentum equation that was first proposed by Euler.

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla P + \rho\mathbf{g}$$

- Often this equation for the momentum conservation and the equation of mass conservation are called Euler's equations for fluids.

- Notice that fluids cover a wide range of phenomena. Depending on the fluid and the conditions it is under; pressure, temperature, velocity, etc. Wether only pressure is important, or also viscosity or if the fluid can be compressed or if the anisotropic nature of the stress tensor is important will vary.

ENERGY CONSERVATION

- Finally there is the equation of energy conservation. In the Lagrangian form it is

$$\rho \frac{Dh}{Dt} = \frac{DP}{Dt} + \nabla \cdot (k \nabla T) + \Phi$$

- where h is the enthalpy, k is the thermal conductivity and Φ is the viscous dissipation function, which is how mechanical energy of flows is converted into heat.
- Like the momentum equation there are many cases where thermal conductivity and/or viscous dissipation are negligible in which case the change in enthalpy is just do to changes in pressure.

FLUID DYNAMICS EXAMPLE

- Let's consider a simple system, governed by Euler's equations (no viscosity, incompressible) and with no external forces. Then are equations for mass and momentum in the Eulerian approach would be

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot (\nabla \mathbf{u}) = \frac{\nabla P}{\rho}$$

- Let us consider a small perturbation in a uniform fluid. So the values of ρ, P and **u** will differ only by small amount from their average values. Then we can expand the quantities by

$$\rho = \rho_0 + \rho_1 \qquad P = P_0 + P_1 \qquad \mathbf{u} = \mathbf{u}_1$$

FLUID DYNAMICS EXAMPLE

- Putting these variables back into the fluid equations gives

$$\frac{\partial \rho_0}{\partial t} + \frac{\partial \rho_1}{\partial t} + \nabla \cdot ((\rho_0 + \rho_1)\mathbf{u}_1) = 0 \qquad \frac{\partial \mathbf{u}_1}{\partial t} + \mathbf{u_1} \cdot \nabla \mathbf{u_1} = \frac{\nabla (P_0 + P_1)}{\rho_0 + \rho_1}$$

- We can now keep only first order terms to linearize the equation. This gives us

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \nabla \cdot \mathbf{u}_1 = 0 \qquad \rho_0 \frac{\partial \mathbf{u}_1}{\partial t} = -\nabla P_1$$

- There zeroth order terms are removed because the zeroth order terms had no motion, u_0=0.
- This makes $\partial \rho_0 / \partial t = 0$ and $\nabla P_0 = 0$.

FLUID DYNAMICS EXAMPLE

- Now let's take a second time derivative of the mass conservation equation.

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \nabla \cdot \mathbf{u}_1 = 0$$

$$\frac{\partial^2 \rho_1}{\partial t^2} + \frac{\partial}{\partial t} \rho_0 \nabla \cdot \mathbf{u}_1 = 0$$

- And let's take the divergence of the momentum conservation equation.

$$\rho_0 \frac{\partial \mathbf{u}_1}{\partial t} = -\nabla P_1$$

$$\nabla \cdot \rho_0 \frac{\partial \mathbf{u}_1}{\partial t} = -\nabla^2 P_1$$

- Substituting the second equation into the first gives

$$\frac{\partial^2 \rho_1}{\partial t^2} - \nabla^2 P_1 = 0$$

EQUATION OF STATE

- In general the fluid equations themselves are not enough to solve for the fluids behavior. One also needs what is called an *equation of state*, which is a relationship between density and pressure in the fluid.
- The ideal gas law is an example of an equation of state. In it pressure is proportional to density.

$$P = c_s^2 \rho$$

- Where we have introduced c_s^2 as the constant of proportionality. We can now substitute this in to our equation to get

$$\frac{\partial^2 \rho_1}{\partial t^2} - c_s^2 \nabla^2 \rho_1^2 = 0$$

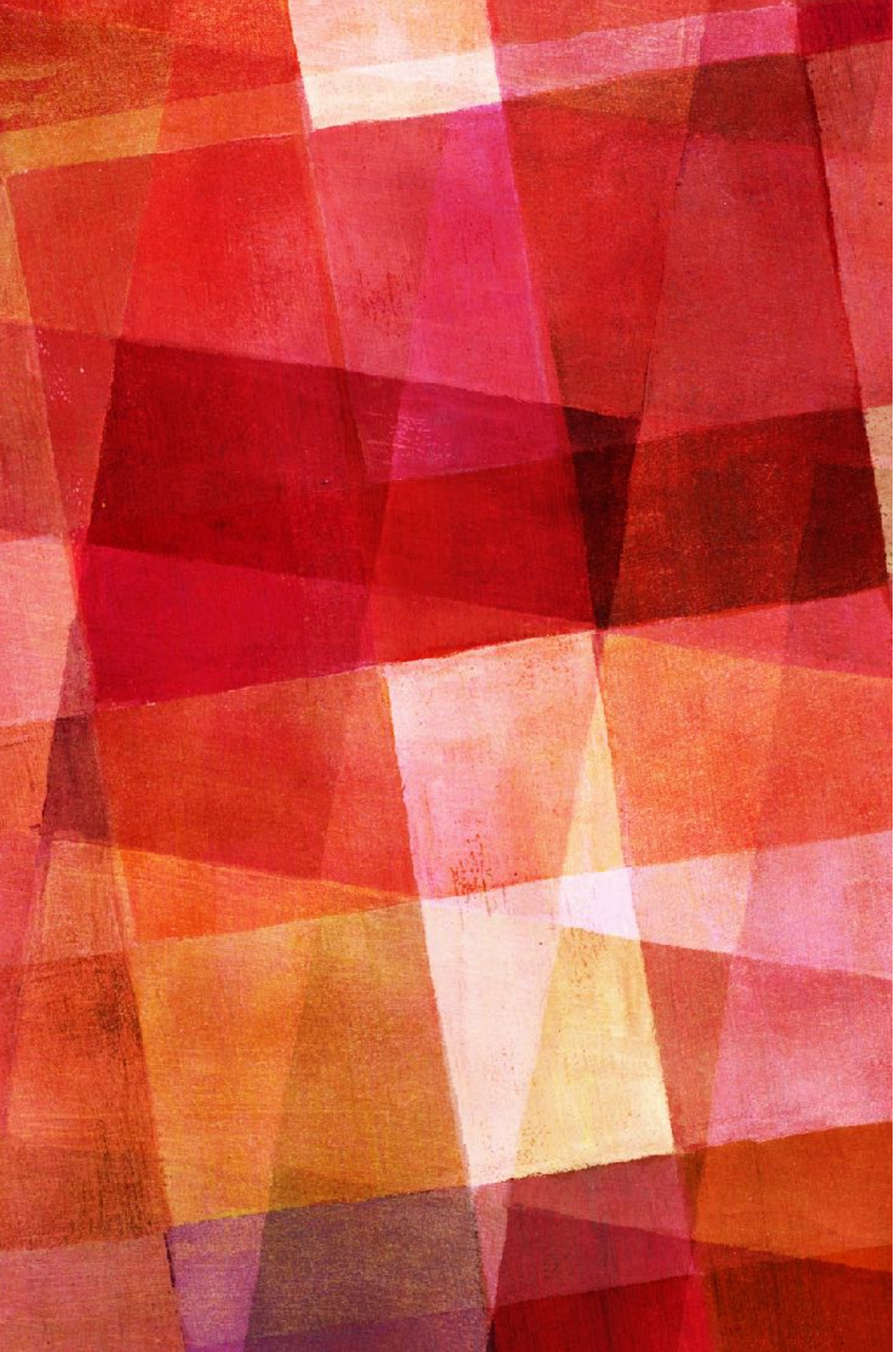
SOUND WAVES

$$\frac{\partial^2 \rho_1}{\partial t^2} - c_s^2 \nabla^2 \rho_1^2 = 0$$

- This is of course just the wave equation and we see that c_s is the sound speed in the fluid. Solution will be of the form

$$\rho_1 = A e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)} \qquad \text{where} \qquad \omega = c_s k$$

- So we find that small perturbations in a uniform at rest fluid will generate sound waves that propagate through the fluid with a speed c_s.
- This is what we expect, but we can see how it comes about from the fluid equations. If the viscosity hadn't been zero then there would have been a damping term and the sound waves would die out over time having their energy go into heating the fluid.



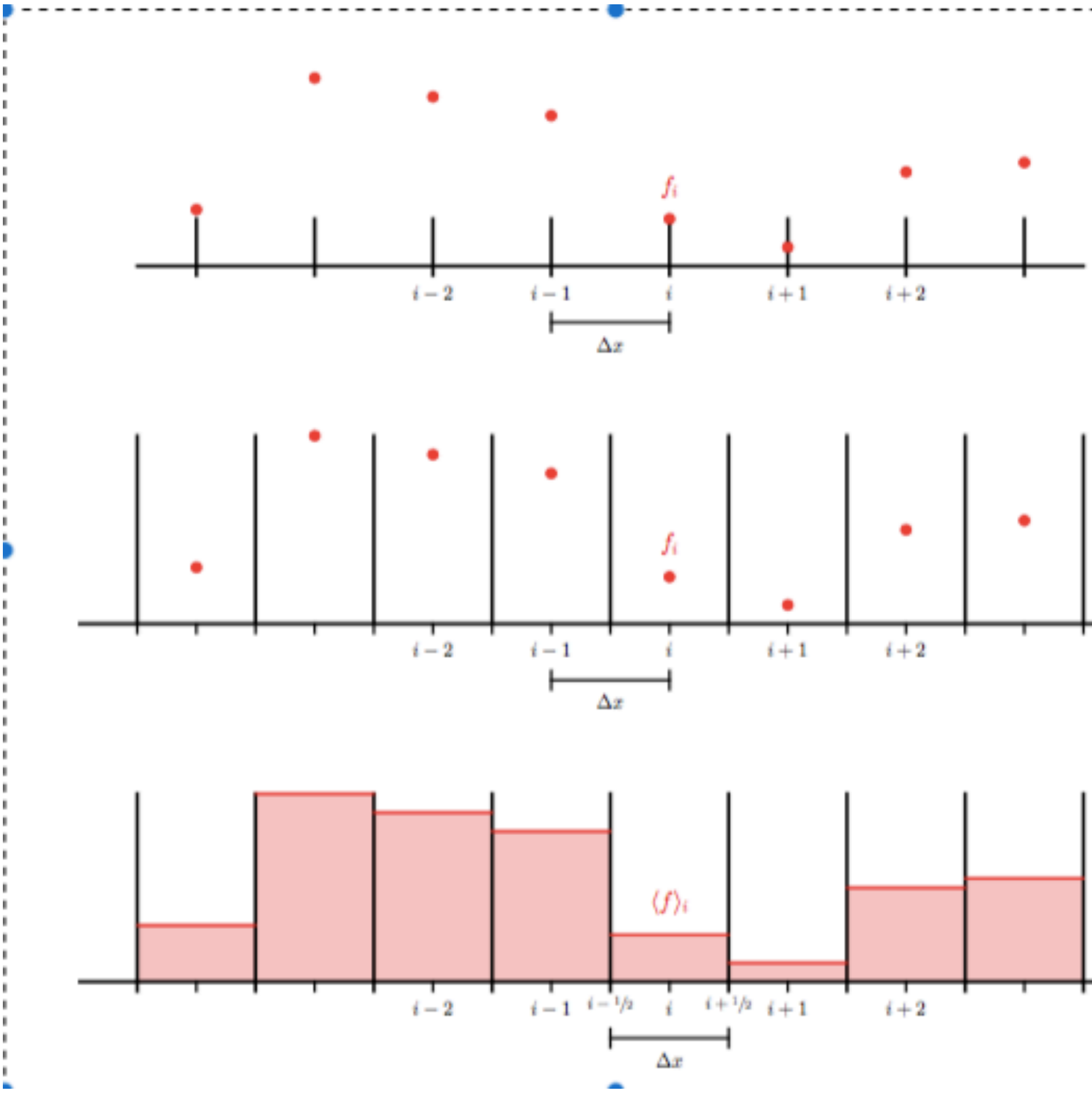
DISCRETIZATION

- The grid
- Advection
- The CFL condition
-

DISCRETIZATION

- We now need to discretize our problem to transform it into something we can solve numerically.
- When we looked at PDEs earlier we focused on the *finite-difference* approach. We discretized the problem by creating a grid and only solving for the values of our function at those grid points.
- Another way to discretize a function is called the *finite-volume* approach. In this case the grid divides our function into volumes and the values at the grid points are the volume averaged value of the function in that cell.
- The *finite-volume* technique is often used for problems where conservation of a quantity is an important feature.

finite difference on the edge or the center of a grid and finite volume



DIFFERENCES

- Calculating derivatives in the finite-volume approach is slightly different if one wants to go higher than 2nd order accuracy.
- To approximate higher order derivatives one first interpolates the value of the function from the mean value in the volume over the number of cells to give the desired accuracy.
- The derivative is then calculated from this fit or spline. For example a fit to three cells is just a parabola and give us the central difference formula we are used to,

$$\frac{\partial f}{\partial x_i} = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1)}}{\Delta x}$$

CONSERVATION

- The finite-volume grid is particularly useful when dealing with conserved quantities. Consider an equation like we have seen for conservation of mass for a fluid

$$\frac{\partial \mathbf{U}}{\partial \mathbf{t}} + \nabla \cdot (\mathbf{F}(\mathbf{U})) = 0$$

- where $\mathbf{U}$ is a vector of quantities and $\mathbf{F}(\mathbf{U})$ is the flux of those quantities. Now if we integrate over a cell volume and normalize by the width of the cell we get

$$\frac{1}{\Delta x} \iiint \frac{\partial \mathbf{U}}{\partial \mathbf{t}} dV = \frac{1}{\Delta x} \iiint \nabla \cdot \mathbf{F}(\mathbf{U}) \mathbf{dV}$$

- but according to the divergence theorem (or Gauss's Law) the right hand side is just the flux through the cells walls. While moving the time derivative outside the integral the left hand side is just the volume average of our quantities U.

$$\frac{d\langle U \rangle}{dt} = \sum_{j=0}^{5} \mathbf{F}(\mathbf{U})|_{\mathbf{side_j}}$$

CONSERVATION

$$\frac{d\langle U\rangle}{dt} = \sum_{j=0}^{5} \mathbf{F(U)}|_{\mathbf{side_j}}$$

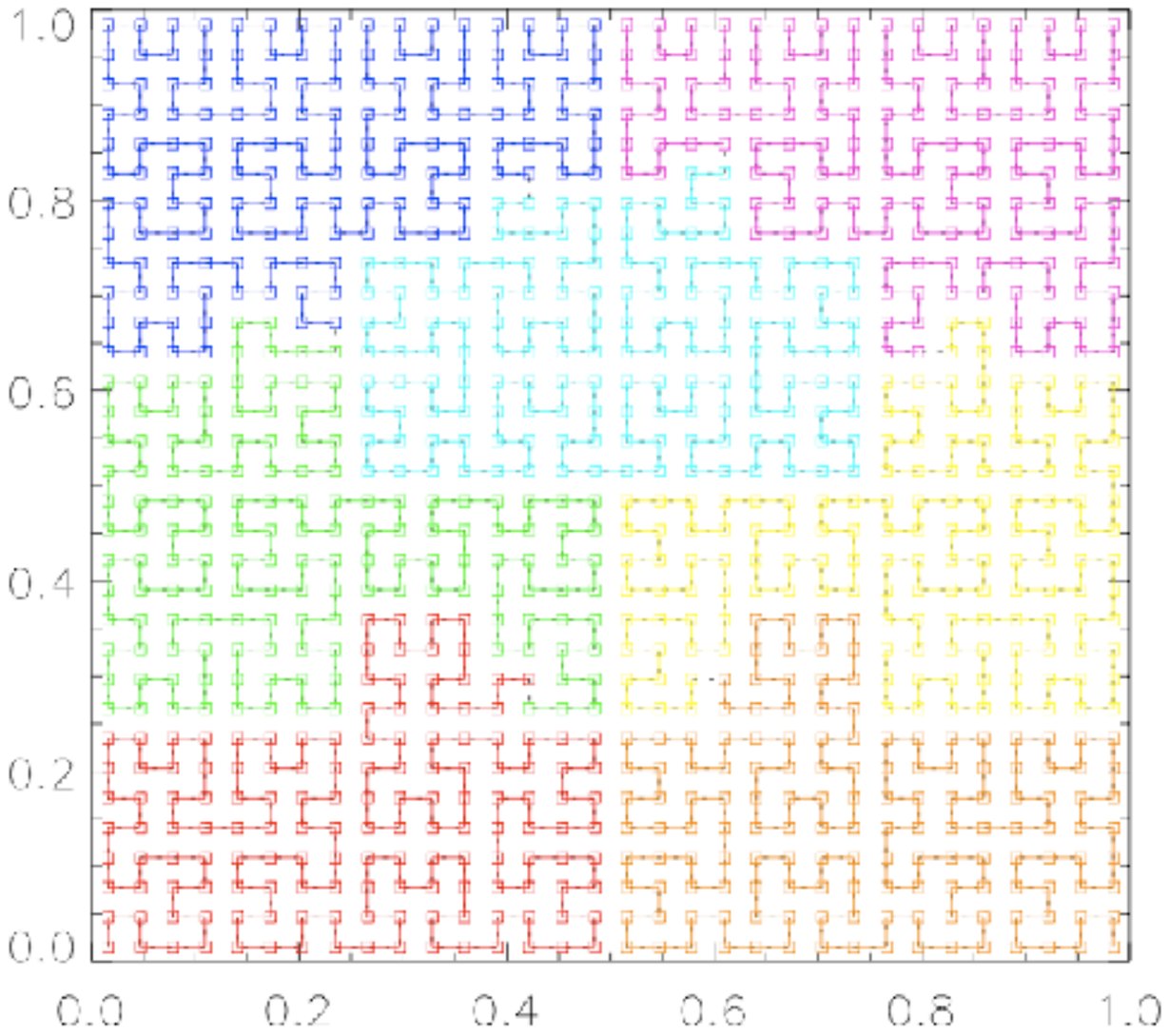
- So when we update the average property in a cell it is determined by the fluxes through the cell boundaries. But the cell boundaries are shared, so the flux lost through a boundary is the flux gained in the next cell.
- This means that to roundoff error the amount of the property is conserved. Whatever is lost from one cell must be gained by other cells.
- This property makes finite-volume very attractive for problems where you are concerned about conserved quantities and since the equations of fluid dynamics are conservation equations finite-volume is one of the favored approaches.

BOUNDARY CONDITIONS

- One issue that arises in finite-volume grids is what happens at the boundary of your grid.
- Since we update our average value based on the fluxes into the cell, what do we do with the end cells?
- The usually solution is to have a layer of ghost cells at the end of our ‘real’ cells. The ghost cells will have flux flow with the rest of the cells, but the values of properties in them are set by boundary conditions. That is not updated like the rest of the cells.
- How the ghost cells are treated is an important issue when using this approach.

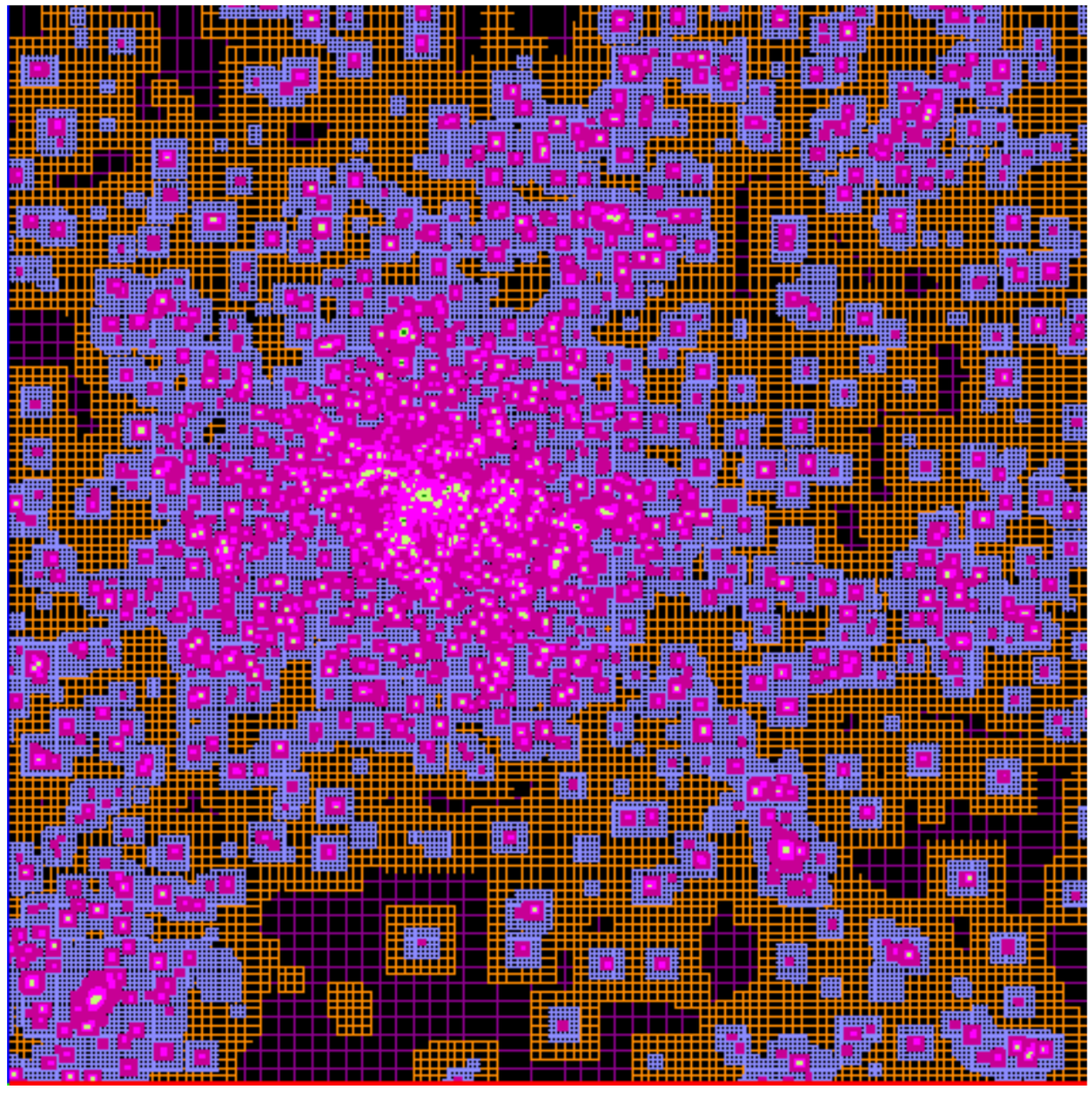
MORE ON GRIDS

- *Domain Decomposition* - Parallelizing a grid can work by breaking it up into domains and then treating each domain on a separate processor. Then the boundary ghost cells get their values from the other domains.
- *Adaptive Mesh Refinement* - Grids can also be extended by adding finer resolution grids based on relevant criteria like the density in the grid. In this way you can have high resolution in some places and low resolution in others.
- *Mapped Grids* - One is also not restricted to rectangular grids. One can map a grid into any shape as long as you know which cell is next to which and the area of the surface between them.
- *Lagrangian Grids* - Also, the grid does not need to be static. One can have the grid move in space, in some way that makes sense to the problem. In this way one can gain many of the advantages of a Lagrangian approach.



➤ *Domain Decomposition*

➤ *Adaptive Mesh Refinement*



ADVECTION

- A physical process whose solutions are similar to what is done for fluid dynamics, but is in general simpler, is advection. A linear advection equation is of the form:

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

- where a is some scalar quantity that gets advected with a velocity u. In this simple form a(x,t) will simply move at the speed u, so a(x'=x+u(t'-t),t') is just a(x,t).
- Trying to solve such an equation numerically using a finite difference method will lead to instabilities like we saw when learning about FTCS (forward-time centered-space).

ADVECTION - FVM

- Instead we can approach the problem using the finite-volume method. Then we want the equation in conservative form

$$\frac{\partial a}{\partial t} + \frac{\partial f(a)}{\partial x} = 0$$

- where f(a) is the flux of a which is just ua in this case. Now to discretize we use a finite volume grid where each cell represents the average volume of the fluid in that cell.

- Integrating over a cell i gives

$$\frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial a}{\partial t}\, dx = -\frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial}{\partial x} f(a)\, dx$$

$$\frac{\partial a}{\partial t} = -\frac{1}{\Delta x}\left([f(a)]_{i+1/2} - [f(a)]_{i-1/2}\right)$$

COURANT CONDITION

- We also need to discretize the time derivative. It can be shown that for the solution to be stable the time step must be less than the time it takes information to cross a cell.

$$\Delta t \leq \frac{\Delta x}{u}$$

- This is called the *Courant-Friedrichs-Lewy* or CFL or just *Courant* condition. It is an extremely important condition in numerical simulations and often is the main issue driving the cost of the simulation.

- One can define a CFL number, C, and express the time step size using that number. C might be 0.7.

$$C = \frac{\Delta t u}{\Delta x} \qquad \Delta t = C\frac{\Delta x}{u}$$

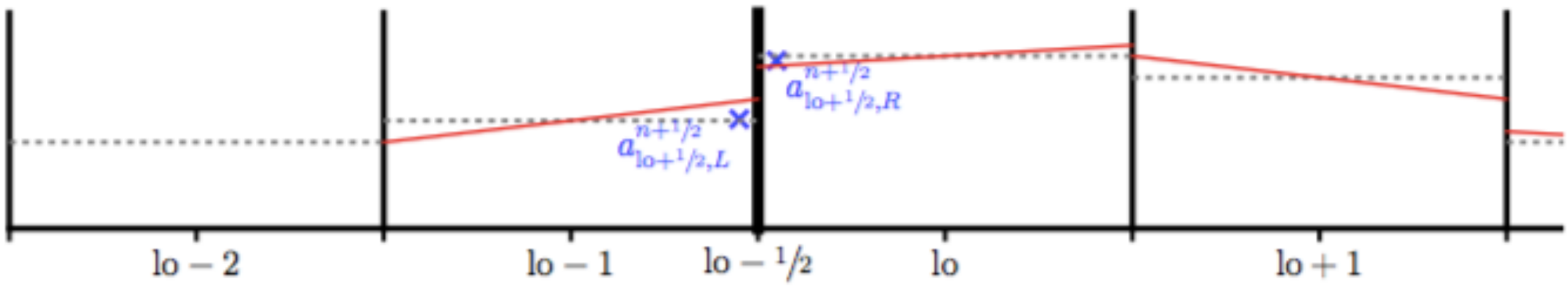
RIEMANN PROBLEM

- So this would give us something like

$$\frac{a_i^{n+1} - a_i^n}{\Delta t} = -\frac{[f(a)]_{i+1/2}^{n+1/2} - [f(a)]_{i-1/2}^{n+1/2}}{\Delta x}$$

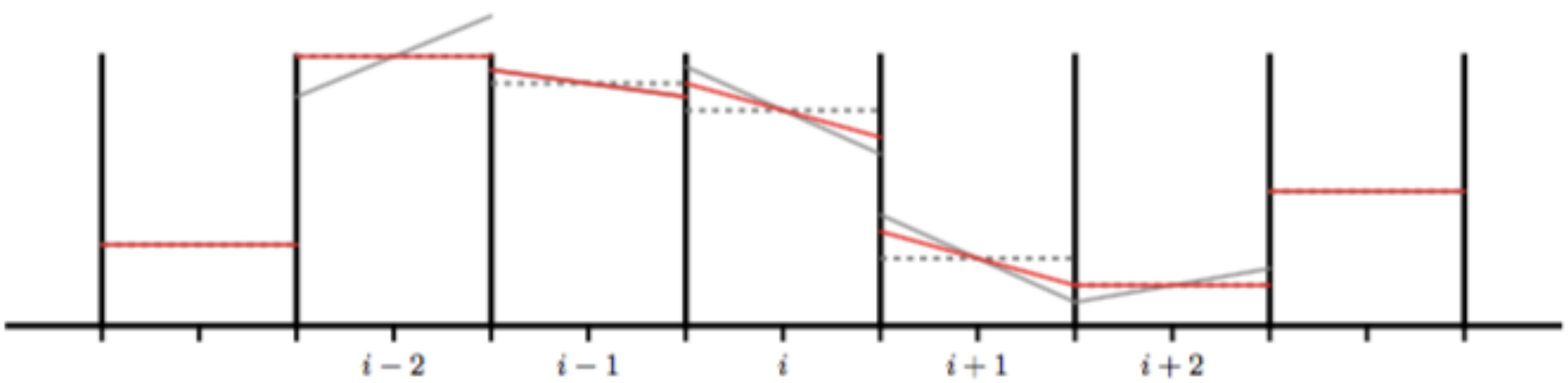
- where we evaluate the fluxes a half time step ahead and n is the number of time steps we have done.

- The right side of the equation, solving for the flux between two piecewise constant data with a single discontinuity is called a Riemann problem. Thus the finite-volume approach always becomes a series of Riemann problems.



LIMITING THE SLOPE

- In order to get a more accurate (higher order) approximation we don't just take the value of a in cell i, but approximate a slope of a to the boundary based on the cells on either side of i. This can be extended to higher order interpolations using more than just neighboring cells.
- It is also common to limit the value of this slope to dampen instabilities. The figure below shows a slope and a limited slope in red.



EULER'S EQUATIONS

- Now let us return to Euler's Equations. While significantly more complicated than the advection equation we will solve them in essentially the same way.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla P = 0$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{u} + P\mathbf{u}) = 0$$

- Written like this we see they look like 3 divergence equations, but are also three nonlinear simultaneous equations. For simplicity let's move to 1D equations.

EULER'S EQUATIONS – 1D

- Then we could write all 3 equations together as a vector

$$\frac{\partial \mathscr{U}}{\partial t} + \frac{[F(\mathscr{U})]}{\partial x} = 0$$

- where

$$\mathscr{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix} \qquad F(\mathscr{U}) = \begin{bmatrix} \rho u \\ \rho u u + P \\ \rho u E + u P \end{bmatrix}$$

- We can then compute the Jacobian of the flux vector and diagonalize it. The eigenvalues are then the speeds at which information propagates through the fluid.
- Discretizing on a finite-volume grid we again have the Riemann problem on the cell interfaces.

GODUNOV SCHEME

- This Riemann problem is much harder to solve, it is nonlinear and involves 3 waves, but there are many methods which we won't detail here.
- With a Riemann solver in place updating our grid becomes

$$\mathscr{U}_i^{n+1} = \mathscr{U}_i^n + \frac{\Delta t}{\Delta x}(F_{i-1/2}^{n+1/2} - F_{i+1/2}^{n+1/2})$$

- This approach to solving the problem is called a Gudunov scheme after the man who proposed it (in 1959).
- It is one of the most popular approaches to solving computational fluid dynamics, though there are many other methods. Some slight alterations while others approach the problem in a completely different framework.

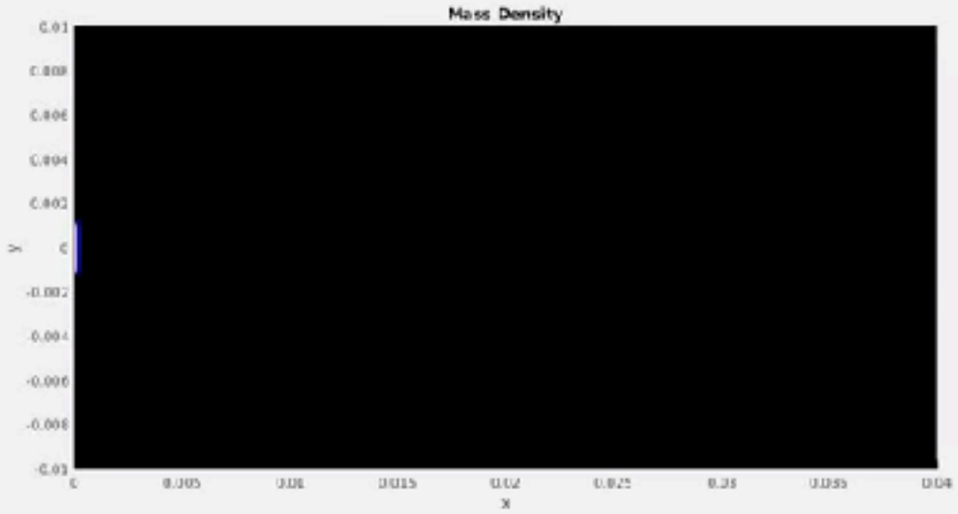
SMOOTH PARTICLE HYDRODYNAMICS

- A completely different approach also widely used in hydrodynamic is to discretize the fluid by mass instead of volume.
- In this case the fluid element in represented by a particle that has a conserved mass and other fluid properties that vary with time.
- The fluid properties are not associated with just one particle, but instead are a smoothed over some number of neighbor particles, usually 32 or more.
- The smoothing kernel can be different functions like a Gaussian for example.

SMOOTH PARTICLE HYDRODYNAMICS

- To determine the fluid properties at a particle's location one finds the N nearest neighbors and then calculates the fluid properties smoothing using the SPH kernel.
- One then solves the fluid dynamic equations to update the flow velocity for that particle and then that particle is advanced according to that calculation.
- This method is explicitly Lagrangian as the particles are moved along the flow lines. It also explicitly conserves mass.
- The method is known to have issues with shock capturing and to create artificial surface tension when one has a multiphase medium.

10.000.000 Fluid Particles


Mass Density
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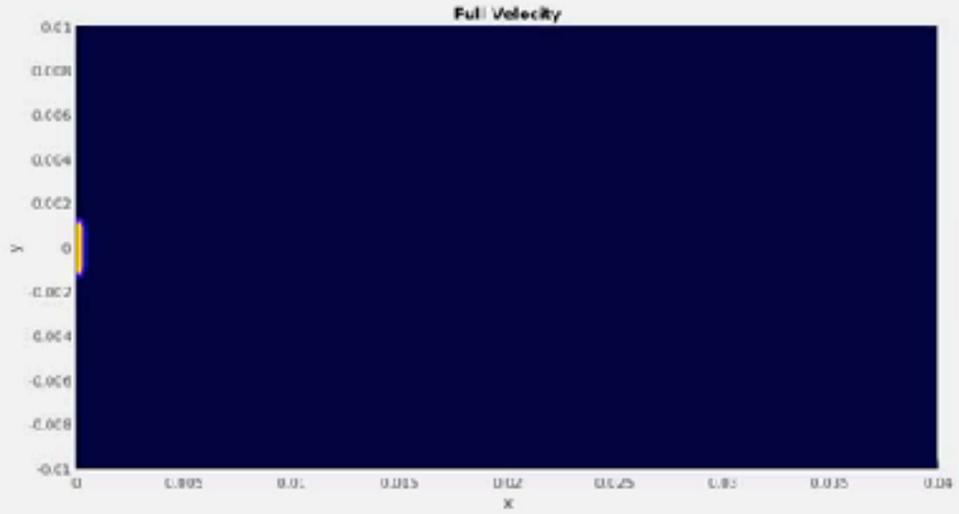
Full Velocity
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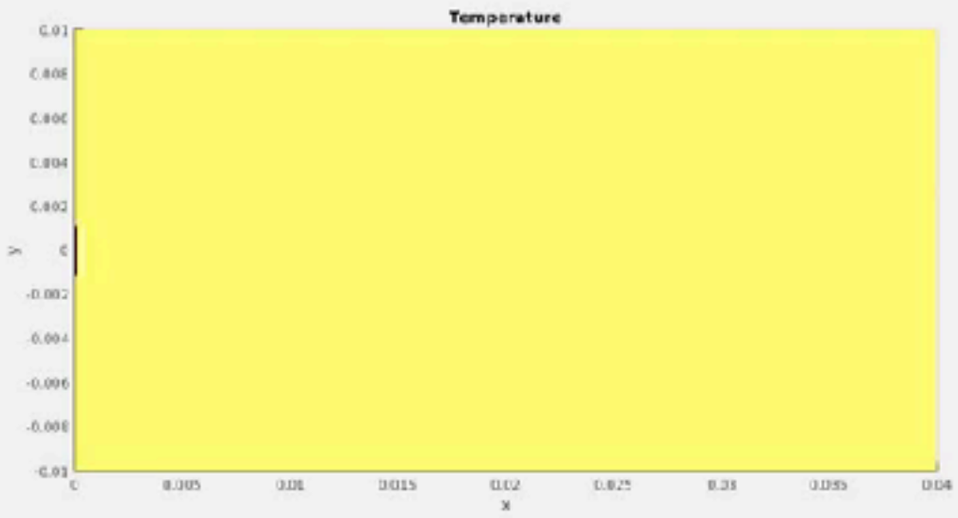
Temperature
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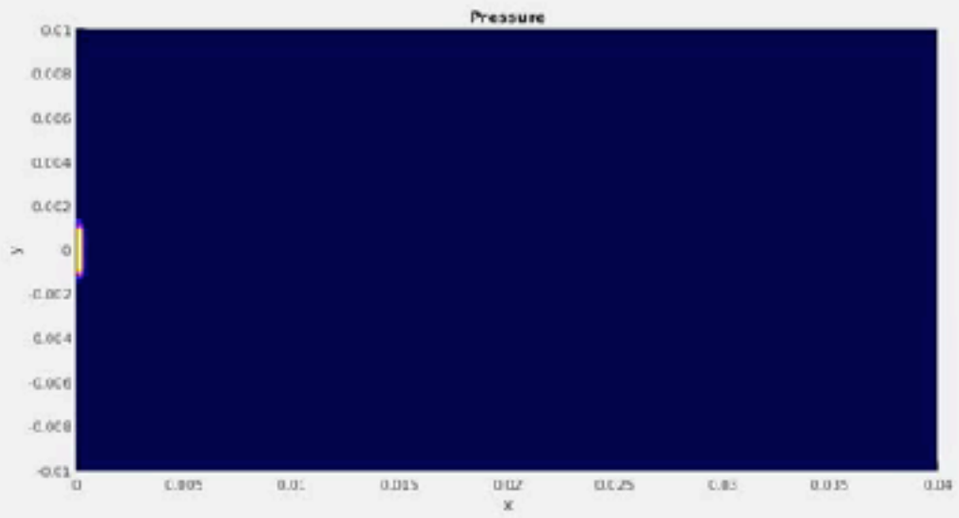
Pressure
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