Computational MHD: Foundations, Uses, and Limitations

Paul Cassak
West Virginia University
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Background figure - Servidio et al., in prep
Outline

• Big Picture
  – Simulations in Plasma Physics
  – Simulation Techniques: PIC vs. Fluid (MHD)
• Numerical Techniques for Fluid Equations
• Examples and Applications
• Pros, Cons, and Pitfalls
• Extensions
A Wide Range of Plasmas

PLASMAS - THE 4th STATE OF MATTER

- Magnetic fusion reactor
- Inertial confinement fusion
- Solar core
- Solar corona
- Lightning
- Solid, liquids, and gasses
- Interstellar space
- Neon sign
- Fluorescent light
- Flames
- Aurora
- Nets

Temperature (°C)

Number Density (Charged Particles / m³)
Applications: Fusion

• Confining hot and dense plasma for a long enough time can provide an essentially endless supply of energy

• Some Issues
  – How should we build a tokamak to make controlled fusion cost effective?
    • That is, what dimensionless parameters should be used?
  – How do turbulence and plasma instabilities affect confinement?
Applications: Space Weather

• Solar eruptions (coronal mass ejections) spew plasma from the solar surface toward the Earth
  – Impacts astronaut safety
  – Disrupts satellites
  – Disrupts communication

• Some issues
  – Can we predict when eruption will occur?
  – How does the Earth’s magnetosphere react to an eruption?

For each application, the physics is far too difficult to understand (exclusively) with pencil and paper - numerical simulations are an absolute necessity!
Coupling of Large/Small Scales

- The systems in question are each much larger than the dynamical length scale of the plasma
  - Turbulence (say, in the solar wind) transfers energy from the large scale to the small scale
  - Magnetic reconnection occurs when oppositely directed magnetic fields interact at a (small!) boundary layer

- Simulations must be big to capture whole system, but have sufficient resolution to also capture small scale physics!
A “Real” Plasma

• Suppose there are $N$ particles and treat each charged particle separately
  – Calculate the force between each particle

\[ m_i \frac{dv_i}{dt} = F_i = q_i \left( E + \frac{v_i \times B}{c} \right) \]

\[ E = \sum_{j \neq i} \frac{q_j}{r_{ij}^2} \hat{r}_j, \quad B = \sum_{j \neq i} \frac{v_j \times E}{c} \]

– For each particle, the fields are a sum over $(N-1)$ particles
– There’s $N$ total particles
– Calculations per time step $\sim N^2$
  • Prohibitively expensive for large $N$!
Particle-In-Cell (PIC) Method

- Forces are due to electric and magnetic fields
  - Define fields on a grid
  - Extrapolate to each particle’s location

- Kinetic Particle in Cell
  - Step fields: Faraday, Ampere Laws (particle quantities averaged to grid)
  - Step particles: Newton’s Law (fields interpolated to particle position)

- PIC can be thought of as a Monte-Carlo technique
  - $E$, $B$ act as fluids
  - Ions, electrons are particles
  - Order $N$, not $N^2$
Realistic Systems in PIC

- Example - the solar corona
  - $n \sim 10^9 / \text{cm}^3$, Vol(single flux tube) $\sim 10^{28} \text{cm}^3$
  - $\Rightarrow N \sim 10^{37}$ particles (per flux tube!)

- Example - the magnetosphere
  - $n \sim 10 / \text{cm}^3$, Vol $\sim 40 \text{R}_E \times 40 \text{R}_E \times 120 \text{R}_E \sim 5.0 \times 10^{31} \text{cm}^3$
  - $\Rightarrow N \sim 5 \times 10^{32}$ particles

- Example - Tokamak
  - $n \sim 10^{13} / \text{cm}^3$, Vol $\sim 2 \text{m} \times 2 \text{m} \times 10 \text{m} \sim 50 \text{m}^3$
  - $\Rightarrow N \sim 5 \times 10^{20}$ particles

- The biggest PIC simulations to date contain $\leq 10^{12}$ particles (Yin et al., 2008)
  - PIC is woefully unable to perform direct numerical simulations of systems of interest in space physics
**Fluid Methods**

- Break up plasma into infinitesimal cells
- Define average plasma properties for each cell (fluid element)
  - Density $n$, velocity $v$, pressure $P$, magnetic field $B$
  - Acceptable provided a sufficient number of particles per cell
- Need equations for how fluid variables change in time
MHD in a slide

• Mass conservation
  – If flow (mass flux $n \nu$) diverges from a point, the density will go down

• Momentum equation
  – Newton’s Law

• Faraday’s Law

• Ohm’s Law
  – a plasma is a perfect conductor, so no electric field can exist in the reference frame of the moving plasma

• Some equation of state
  – Often adiabatic ($P / n^\gamma = \text{const.}$) or isothermal ($P = n T$)

MHD in a slide

- Mass conservation

\[ \frac{\partial n}{\partial t} = -\nabla \cdot (nv) \]

- Momentum equation

\[ m_i n \frac{dv}{dt} = -\nabla P + \frac{J \times B}{c} \]

- Faraday’s Law

\[ \frac{\partial B}{\partial t} = -\nabla \times E \]

- Ohm’s Law

\[ E = \frac{-v \times B}{c} \]

- Some equation of state

\[ \frac{d}{dt} \left( \frac{P}{n^\gamma} \right) = 0 \]

These are equations for how \( n, v, B, P \) advance in time!

Very straight-forward to solve numerically!
Simulating Fluid Plasmas

• Define fluid quantities ($n, v, B, P$) on a grid cell
• The dynamical equations tell us how to step forward fluid quantities in time
  – For example, can use data in nearby cells to estimate spatial derivatives
• Initial Value Problem
  – You give me the system initially (at $t = 0$), and I’ll tell you how it will behave in the future (at $t_1 = \Delta t$). Then, I’ll tell you at $t_2 = t_1 + \Delta t$ and so on.
MHD Properties

• There are three and only three waves available
  – fast and slow magnetosonic waves and shear Alfven waves
• Forces are (relatively) easy to understand
  – magnetic tension, magnetic pressure, gas pressure
• Plasma stuck to magnetic field lines (frozen-in)
• Energy is conserved perfectly (no dissipation)

• MHD is good for
  – Large scales (compared to ion gyroradius $\rho_i$)
  – Slow motions (compared to cyclotron times $\Omega_{ci}^{-1}$)
  – It breaks down when motions are fast or on at small lengths

Good news and bad news:
MHD contains less physics than PIC
Realistic Systems in MHD

- Can estimate number of grid cells needed to resolve down to ion gyroradius (where MHD breaks down)
- Example - the solar corona
  - \( \text{Vol (single flux tube)} \sim 10^{28} \text{ cm}^3, \rho_i \sim 1 \text{ m} \)
  - \( \Rightarrow (\text{Vol} / \rho_i^3) \sim 10^{22} \text{ cells (per flux tube)!} \)
- Example - the magnetosphere
  - \( \text{Vol} \sim 2.6 \times 10^{26} \text{ cm}^3, \rho_i \sim 70 \text{ km} \)
  - \( \Rightarrow (\text{Vol} / \rho_i^3) \sim 8 \times 10^{11} \text{ cells} \)
- Example - Tokamak
  - \( \text{Vol} \sim 50 \text{ m}^3, \rho_i \sim 10 \text{ cm} \)
  - \( \Rightarrow (\text{Vol} / \rho_i^3) \sim 5 \times 10^4 \text{ grid cells} \)
- My runs use \( \leq 10^7 \) cells, I’ve seen up to \( \sim 10^9 \)
  - MHD isn’t much better than PIC at getting realistic systems!
  - The estimate here only marginally resolve the gyroscale; actually need to go lower (and capture more physics!)
What do we do?

• Except for few examples where direct numerical simulations (with realistic parameters) can be completed, simulations (fluid and PIC) do not attempt to faithfully reproduce a real system
  – Rather, we study
    • systems with the “relevant” parameters similar to real systems,
    • trends in how results change when a parameter is changed (scaling) with the idea of extrapolating to real systems,

• MHD simulations are useful for large systems where dynamics is slow
  – Solar corona (?), earth’s magnetosphere (?)
  – Studying particular processes (turbulence, reconnection, …)

• People who use MHD are either
  – old and too stubborn to learn a more complete technique or
  – are trying to simplify a difficult problem by taking out as much physics as possible to begin with (with the idea of going back to more realistic models later)
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  - Simulation Techniques: PIC vs. Fluid (MHD)
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Techniques

- Explicit vs. Implicit
- Finite difference vs. Finite volume
- Real space vs. Spectral/Pseudo-spectral
Explicit Finite Difference

- Reference - Numerical Recipes, Press et al.
- Forget about MHD and just consider a more simple "convection equation":
  \[
  \frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x}
  \]
  - The exact solution is \[u(x,t) = f(x - vt)\]
    - This is a wave that simply travels without changing shape

- How to code in?
  - Simplest approach:
    - Called FTCS (Forward Time Centered Space)
    - Here, \(j\) refers to spatial cell and \(n\) refers to time step
    - Makes sense, but it doesn’t work!

\[
\frac{\partial u}{\partial t} \rightarrow \frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t}
\]
\[
\frac{\partial u}{\partial x} \rightarrow \frac{u_{j+1}^{n} - u_{j-1}^{n}}{2\Delta x}
\]
Von Neumann stability analysis

• “Discretized” convection equation becomes

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

• Consider a given Fourier mode in the system

$$u_j^n = u^n e^{ikx}$$

• Plug in and simplify

$$\frac{u_j^{n+1} e^{ikx} - u_j^n e^{ikx}}{\Delta t} = -v \frac{u^n e^{ik(x+\Delta x)} - u^n e^{ik(x-\Delta x)}}{2\Delta x}$$

$$u_j^{n+1} = u^n - \frac{v\Delta t}{2\Delta x} u^n \left(e^{ik\Delta x} - e^{-ik\Delta x}\right)$$

$$u_j^{n+1} = u^n \left[1 - i \frac{v\Delta t}{\Delta x} \sin(k\Delta x)\right]$$
Von Neumann stability analysis

• Then,
  \[
  \frac{u^{n+1}}{u^n} = 1 - i \frac{v \Delta t}{\Delta x} \sin(k \Delta x) = \sqrt{1 + \left(\frac{v \Delta t}{\Delta x}\right)^2 \sin^2(k \Delta x)} \geq 1
  \]

• Therefore, for any \( k \), the amplitude of the “wave” grows in time, and the code will crash! The scheme is said to be “unconditionally unstable.”

• Try this instead - let \( u_j^n \) in time derivative be given by its average over the next two cells

  \[
  u_j^{n+1} = u_j^n - \frac{v \Delta t}{2 \Delta x} \left( u_{j+1}^n - u_{j-1}^n \right)
  \]

  \[
  \rightarrow u_j^{n+1} = \frac{1}{2} \left( u_{j+1}^n + u_{j-1}^n \right) - \frac{v \Delta t}{2 \Delta x} \left( u_{j+1}^n - u_{j-1}^n \right)
  \]

• This is called the Lax method or Lax scheme
Courant Condition

• A von Neumann stability analysis shows that the scheme is stable (i.e., \(|u^{n+1}/u^n| \leq 1\) for all \(k\)) if

\[
\frac{v \Delta t}{\Delta x} \leq 1
\]

• This is called the “CFL condition” (Courant-Friedrichs-Levy), or just the “Courant condition”
  – Physically, it means that for a given grid size \(\Delta x\), the time step \(\Delta t\) must be small enough that no signal can travel more than a grid cell in a single time step
    • If time step is too large, there are problems with causality, and the code crashes!
  – All explicit fluid simulations, independent of scheme, must always be run with a time step satisfying the Courant condition
    • This puts a limit on the amount of resources necessary for a given calculation
“Numerical” Dissipation

• An important realization - the Lax scheme equation can also be written as

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \quad (\text{FTCS})
\]

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \frac{1}{2} \left( \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta t} \right) \quad (\text{Lax})
\]

• The Lax scheme can be thought of as the FTCS expression for the governing equation

\[
\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x} + D \frac{\partial^2 u}{\partial x^2}
\]

where \( D = \Delta x^2 / 2 \Delta t \). The extra term describes diffusion!

– So, one cannot perform pure MHD simulations! Artificial (aka numerical) diffusion must be included to make the scheme stable.

– One must remember when doing MHD simulations that there is diffusion at the grid scale whether one wants it or not!
Convection - Leapfrog

• Instead of forward in time, do centered in time (keeping space as is)

\[
\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = -v \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \quad (CTCS)
\]

– This is an example of a “leapfrog” technique
One needs information about the previous \textit{two} time steps in order to calculate the next one.

• Can think of it as “predictor-corrector” scheme in which one steps from \textit{n-1} time step to \textit{n+1} time step by calculating \textit{n} time step first, then using that information to calculate the \textit{n+1} step.

– Can show stability criterion is again the Courant condition.
Back to MHD

- This is essentially the technique used in the MHD code I run (F3D; Shay et al., 2004)
  - (Trapezoidal) Leapfrog in time,
    fourth order finite difference in space

- The difference is that instead of some parameter $v$ in the convection equation, the wave speed limiting the time step comes from the phase speed of the waves in the system
  - Thus, the Courant condition implies that

$$\frac{v_{\text{fastest}} \Delta t}{\Delta x} \leq 1$$

where $v_{\text{fastest}}$ is the fastest wave speed in the system (the fast magnetosonic speed for MHD)
Example - Magnetic Reconnection

- Black - magnetic field lines
- Color - out-of-plane current
- Field lines break apart at small scales

- Cassak and Shay, 2007
  - Resistive MHD simulations (explicit resistivity $\eta$ included)
  - Two dimensional
  - 4096 x 2048 cells
  - Grid cell $\Delta x = 0.1$
Implicit Finite Difference

• When we did FTCS, why did we choose space derivative at known time step instead of unknown time step? If we choose unknown,
\[
\frac{\partial u}{\partial t} = \frac{u_{j+1}^{n+1} - u_j^n}{\Delta t} \\
\frac{\partial u}{\partial x} \to \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x}
\]

• This scheme is called “implicit.” One solves the system by writing the final data as a matrix times the initial data and solve for data from all time steps simultaneously. This is done with matrix inversion.

• One can show using a von Neumann type stability analysis that the scheme is stable for large time steps
  – Not constrained to use time step smaller than Courant condition!
  – However, the results may not be as accurate as an explicit scheme
Finite volume

• Finite volume is very similar to finite difference
  
  - Write equation in conservative form
    \[
    \frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x} \Rightarrow \frac{\partial u}{\partial t} \approx - \left( \frac{\partial}{\partial x} (vu) \right) \Rightarrow \frac{\partial u}{\partial t} = - \frac{\partial}{\partial x} f
    \]
    Time derivative \(=\) spatial derivative (divergence) of a flux
  
  - Then discretize the flux at the half-cells
    \[
    \frac{u_j^{n+1} - u_j^n}{\Delta t} = - \frac{f_{j+1/2}^n - f_{j-1/2}^n}{\Delta x}
    \]
    This method explicitly enforces that conservation of plasma quantities is preserved.
  
• More easily extended to non-rectangular geometries
Spectral Method

- Expand solution in series of a given basis function (Fourier or Chebyshev, for example)
  \[ u(x,t) = \sum_{n=-\infty}^{\infty} u_n(t)e^{ik_nx} \]
- Apply governing equation to the series solution, which converts PDE to a set of ODEs for the coefficients of the expansion
  \[
  \frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x} \\
  \sum_{n=0}^{\infty} \frac{du_n(t)}{dt} e^{ik_nx} = -v \sum_{n=0}^{\infty} ik_n u_n(t)e^{ik_nx} \\
  \frac{du_n(t)}{dt} = -(ik_n v) u_n(t)
  \]
- Solve using your favorite ODE solver, such as Runge-Kutta 4
  - An infinite series would be exact; only a finite number of terms can be coded in
- Better accuracy for less resources than finite difference
Pseudo-spectral Method

• Fourier transform in space, converting to simple ODE in time

\[
\frac{du}{dt} = -v \frac{du}{dx}
\]

\[
\Rightarrow \frac{d\hat{u}(k,t)}{dt} = -ikv\hat{u}(k,t)
\]

• Easy to integrate in time (by hand, not by code)

\[
\hat{u}(k,t) = e^{-ikvt}\hat{u}(k,0)
\]

• Inverse Fourier transform in space

\[
u(x,t) = F^{-1}\left[e^{-ikvt}\hat{u}(k,0)\right]
\]

• Simulation requires only Fourier Transforms, which can be done very quickly (Fast Fourier Transform - FFT)

• Drawback - all information is global, noise is spread non-causally to whole grid
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Solar Applications

- Flux emergence
- Abbett, Berkeley
- Spectral in horizontal direction, finite difference in vertical
- In time, uses operator splitting (convection and diffusion), “semi-implicit”

Abbett and Fisher, 2003
Coronal Mass Ejection Initiation

- MacNiece, NASA Goddard
- Flux corrected transport (more complicated finite volume technique)

MacNiece et al., 2004
Turbulence

- MHD Turbulence (Servidio, Univ. Delaware)
- Fourier Pseudo-spectral in space
- Runge-Kutta 4 in time
Astrophysics

- Zeus (Stone, Princeton)
- Convection in Black Hole Accretion Disk
Tokamaks

- NIMROD (Sovinec, Univ. Wisconsin)
- Non-Ideal Magnetohydrodynamics with Rotation - Open Discussion
- Finite element in two dimensions
- Pseudo-spectral in third
- Implicit in time

https://nimrodteam.org/
Global Magnetosphere

- Open GGCM (Raeder, UNH)
- Explicit time integration
- Finite difference in space (conservative and flux-limited)
- Yee grid to preserve div B
- Couples to a model of ionosphere
- Resolution only down to 100 km
Adaptive Mesh

• Powerful technique in which the grid scale is changed during run-time to ensure higher resolution in the regions that need it
  – (Berger, Oliger, Colella)

c.t.gsfc.nasa.gov/insights/vol13/tele.htm
Global MHD Simulations

- BATS-R-US (Univ. Michigan)
- Block Adaptive Tree Solarwind Roe Upwind Scheme
- MHD, finite volume, adaptive mesh
- Amazing resolution! (Not anywhere near good enough!, clearly doesn’t get the physics right)
CCMC

• Community Coordinated Modeling Center
• Operated by NASA-Goddard
• Collection of open codes
  – Solar, Heliospheric, Magnetospheric, Ionospheric
• Can request codes to run simulations!
• http://ccmc.gsfc.nasa.gov/
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MHD Cheaper Than PIC

• It is much less expensive to do a run in MHD than the same run with PIC
  – For MHD, you set up a grid and carry around seven variables \((n, v, B)\) at each grid point
    • For 1000 x 1000 grid, that’s 7,000,000 pieces of data per time step
  – For PIC, you have position and velocity of all particles, plus fields \((E, B)\) at each grid point
    • For 1000 x 1000 grid with \(10^9\) particles, that’s
      \(6 \times 10^6 + 6 \times 10^9 \sim 6 \times 10^9\) pieces of data per time step
    • Much more data, much more storage necessary in PIC!
PIC Noisier Than MHD

• PIC codes are typically very noisy
  – Relatively few particles being simulated means worse statistics
  – Smoothing over space and/or time necessary to extract data
• MHD codes are very clean

Hybrid

Hall-MHD
Parallelization

• Modern large simulations are carried out on multiple processing units simultaneously
  – A code that takes one year on one processor takes ~ one day on 365 processors!

• The process taking the most time for explicit MHD simulations is simply the time evolution
  – More processors implies more communication between processors, which slows things down
  – Need to be creative to get fluid code to “scale” to many processors
  • In contrast, PIC codes scale very well, regularly going up to thousands of processors (less communication needed)