# Computational Methods for Fluids (Gyro) Kinetic Equations. Lecture I

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## Alternative Title

The Lively Art of Constructing Discrete Plasma Universes

# Computational Plasma Physics: Uniquely Challenging

Vast majority of plasma physics in contained in the Vlasov-Maxwell equations that describe self-consistent evolution of distribution function $f(\mathrm{x}, \mathrm{v}, t)$ and electromagnetic fields:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathrm{x}} \cdot (\mathrm{v} f_s) + \nabla_{\mathrm{v}} \cdot (\mathrm{F}_s f_s) = \left(\frac{\partial f_s}{\partial t}\right)_c$$

where $\mathrm{F}_s = q_s/m_s(\mathrm{E} + \mathrm{v} \times \mathrm{B})$. The EM fields are determined from Maxwell equations

$$\frac{\partial \mathrm{B}}{\partial t} + \nabla \times \mathrm{E} = 0$$
$$_0\mu_0 \frac{\partial \mathrm{E}}{\partial t} \quad \nabla \times \mathrm{B} = \quad \mu_0 \sum_s q_s \int_{\infty}^{\infty} v f_s \, d\mathrm{v}^3$$

Theoretical and computational plasma physics consists of making extensions/approximations and solving these equations in specific situations.

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- Highly nonlinear with the coupling between fields and particles via currents and Lorentz force. Collisions can further complicate things
- High dimensionality and multiple species with large mass ratios: 6D phase-space, $m_e/m_p = 1/1836$ and possibly dozens of species.
- Enormous scales in the system: light speed and electron plasma oscillations; cyclotron motion of electrons and ions; fluid-like evolution on intermediate scales; resistive slow evolution of near-equilibrium states; transport scale evolution in tokamak discharges. 14 orders of magnitude of physics in these equations!

# Goals and Outline

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Goal of these lectures is to introduce modern concepts in computational plasma physics, specially with a view towards connecting *continuous* and *discrete* properties of the equations.

- **Part 1**: Physics that should be preserved in the discrete system. Indirect properties and going beyond accuracy and order of schemes.
- **Part 2:** Schemes for fluid and (gyro) kinetic equations. Mostly focussed on Finite-Volume (FV) schemes for multi-fluid equations, and advanced discontinuous Galerkin (DG) for (gyro) kinetic equations.

Treat kinetic and multifluid, multimoment equations as PDEs. Not a talk on PIC methods! (See work by H. Qin, P. Morrison et al on modern structure preserving schemes).

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- The goal here is the numerical method itself: what are its properties? Does it faithfully represent the underlying physics? Does it run efficiently on modern computers? Research into modern numerical methods (including structure preserving methods) fall into this category.
- Usually, besides the fun of solving complex equations, we wish to gain deeper understanding of underlying physics. **Some theoretical questions can only be answered with computer simulations.**

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As a tool for applications:

- The second reason to care is that computational physics provides tools to understand/design experiments or observations.
- Large number of routine calculations are needed to build modern experiments (heat-transfer, structural analysis, basic fluid mechanics, equilibrium and stability calculations, etc). **Such routine calculations are no longer cutting edge research topics.**

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However, today strong need to be at **intersection of cutting-edge computational physics and critical applications**: E.g: More than 6 billion are invested in private fusion efforts; billions more in public efforts.

# Exploring the Fusion Design Space

What is needed to explore or "confine" the design space for the crowded space of fusion concepts?

- Unfortunately, neither the physical models or the numerics are fully developed yet to understand *burning plasma regime*. Enormous scales, hairy plasma-material-interaction and zoo of possible instabilities.

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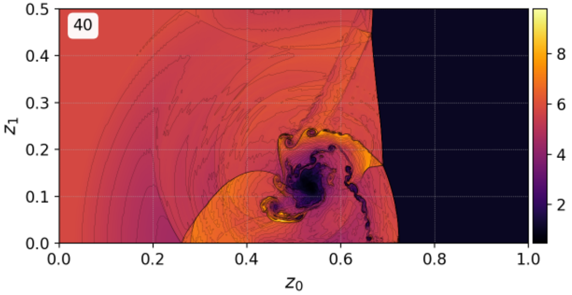
Two approaches:

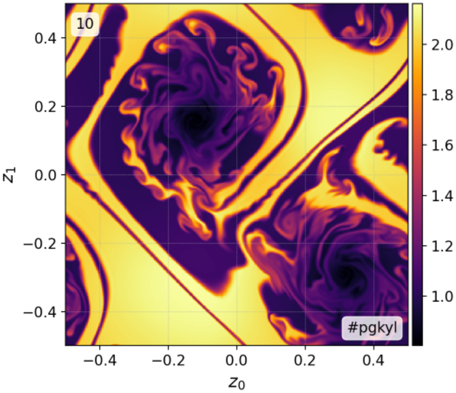
- Do calculations with first-principles models on the large computers. Required to do detailed physics studies
- Do many smaller calculations in an *optimization loop* to confine the design space. Run occasional large calculations to verify.

Each of these approaches needs development of appropriate models, and fast numerical methods on modern hardware architecture. Put everything in an optimization loop.

# Setting the Stage: Shock-Bubble Interactions



# Setting the Stage: Kevin-Helmholtz Instability



## The Ultimate Discrete Scheme (UDS)

A hypothetical "Ultimate Discrete Scheme" must possesses the following three properties

- **Robustness** The scheme must be *robust*: capture shocks, maintain positivity, preserve monotonicity, satisfy involutions (divergence constraints), properly preserve energy partition.
- **Accuracy** Provide low dissipation for smooth high-$k$ modes to properly simulate turbulence. Converge quickly to give accurate results when needed
- **Efficiency** Run rapidly for modest resolutions. Do interesting physics on a laptop. Use GPUs and other hardware accelerators for larger simulations. Do 1000s of simulations.

Sadly, such a scheme does not exist! Many of the goals are contradictory.

# No Free Lunch Principle

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There is no *unique* discrete system of equations corresponding to a given system of continuous equations. No discrete system is perfect and a method that works well in one situation may not work well in others.

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"All numerical methods suck, though some suck less than others. Make sure your method sucks less that the competition"

# Many approximations developed over the decades

Modern computational plasma physics consists of making justified approximations to the VM system and then coming up with efficient schemes to solve them.

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- Many fluid approximations have been developed to treat plasma via low-order moments: extended MHD models; multimoment models; various reduced MHD equations

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- Major recent theoretical development in plasma physics is the discovery of gyrokinetic equations, an asymptotic approximation for plasmas in strong magnetic fields. Reduces dimensionality to 5D (from 6D) and eliminates cyclotron frequency and gyroradius from the system. Very active area of research.
- Many fluid approximations have been developed to treat plasma via low-order moments: extended MHD models; multimoment models; various reduced MHD equations
- Numerical methods for these equations have undergone renaissance in recent years: emphasis on *memetic* schemes that preserve conservation laws and some geometric features of the continuous equations. Based on Lagrangian and Hamiltonian formulation of basic equations. Very active area of research.

# Integrating kinetic effects in fluid models

- For physically accurate simulations of various fusion machines, its important to **go beyond resistive and Hall-MHD**.
- Traditional approach has been to use a generalized Ohm's law, adding physics to it in a piecemeal fashion.
- However, this approach has limited success, and in particular, there is no systematic way to add important collisionless kinetic effects in a self-consistent and numerically tractable manner.
- A major challenge in the fusion and other applications is that the **plasma is nearly collisionless**, and that the **magnetic fields (external coils, planetary dipole) add a preferred direction**, adding significant anisotropy to the system.

# Alternative is to use multi-fluid moment models

- In this approach we take moments of the Vlasov equation, truncating the moment sequence using a closure.
- The interaction between species is via electromagnetic fields, which are evolved using Maxwell equations (retaining displacement currents)
- This approach allows natural and self-consistent inclusion of **nite electron inertia, Hall currents, anisotropic pressure tensor and heat flux tensor**.
- Even though the multi-fluid moment equations contain physics all the way from light waves and electron dynamics to MHD scales, by use of advanced algorithms very efficient and robust schemes can be developed, **allowing us to treat a sequence of increasing delity models in a uniform and consistent manner**.

# Sequence of models with 5, 10 and 20 moments

Taking moments of Vlasov equation leads to the *exact* moment equations listed below

$$
\begin{aligned}
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(n u_j) &= 0 \\
m\frac{\partial}{\partial t}(n u_i) + \frac{\partial \mathcal{P}_{ij}}{\partial x_j} &= nq(E_i + \epsilon_{ijk} u_j B_k) \\
\frac{\partial \mathcal{P}_{ij}}{\partial t} + \frac{\partial \mathcal{Q}_{ijk}}{\partial x_k} &= nq u_{[i} E_{j]} + \frac{q}{m}\epsilon_{[ikl}\mathcal{P}_{kj]} B_l \\
\frac{\partial \mathcal{Q}_{ijk}}{\partial t} + \frac{\partial \mathcal{K}_{ijkl}}{\partial x_l} &= \frac{q}{m}(E_{[i}\mathcal{P}_{jk]} + \epsilon_{[ilm}\mathcal{Q}_{ljk]} B_m)
\end{aligned}
$$

In the **ve-moment** model, we assume that the pressure is isotropic $P_{ij} = p\delta_{ij}$. For the **ten-moment** model, we include the time-dependent equations for all six components of the pressure tensor, and use a closure for the heat-flux. In the **twenty-moment** model, we evolve all ten components of the heat-flux tensor, closing at the fourth moment.

# Planetary Scale Simulations Are Now Possible!

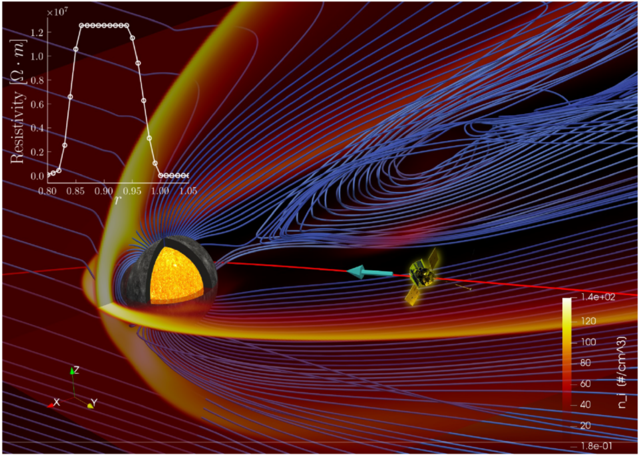
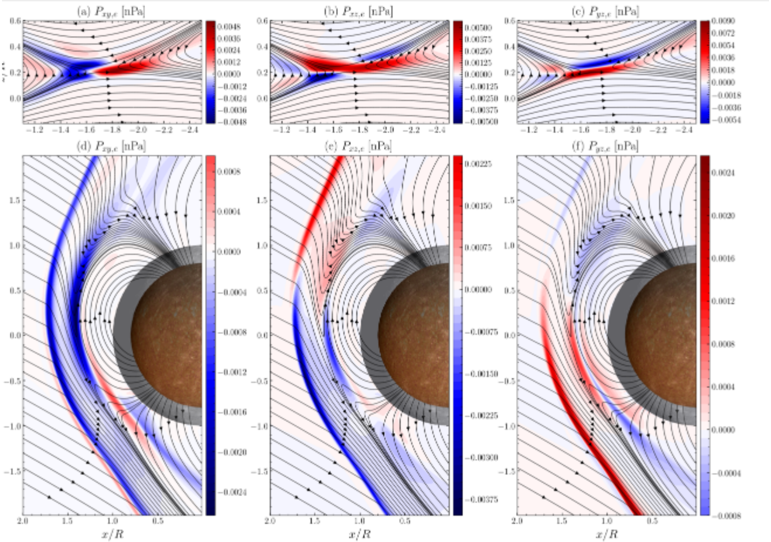



Figure: Ten-Moment Simulation of Mercury's Magnetosphere (Dong et. al. GRL, **46**, 2019

# Reconnection On Mercury's Night and Day Sides



# Earth-Scale Simulations Are "Almost" Possible

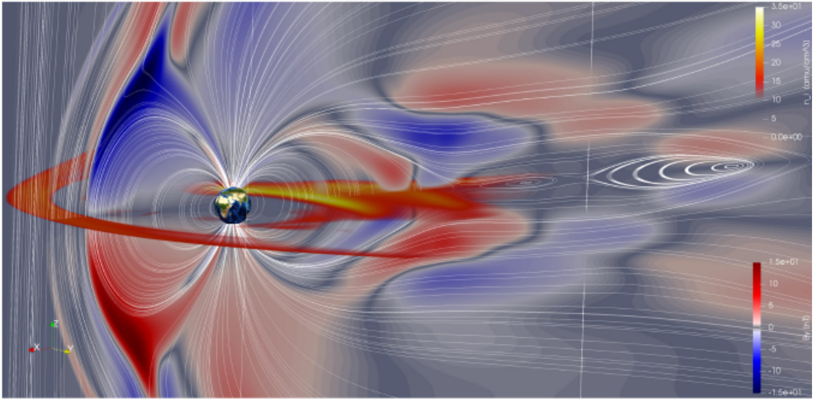


Figure: Ten-Moment simulation of Earth's magnetosphere shows extended night-side current sheet, just after a disruption driven by ballooning instability. Wang et. al. JCP **415**, 2020

# More Planetary Magnetospheres: Uranus

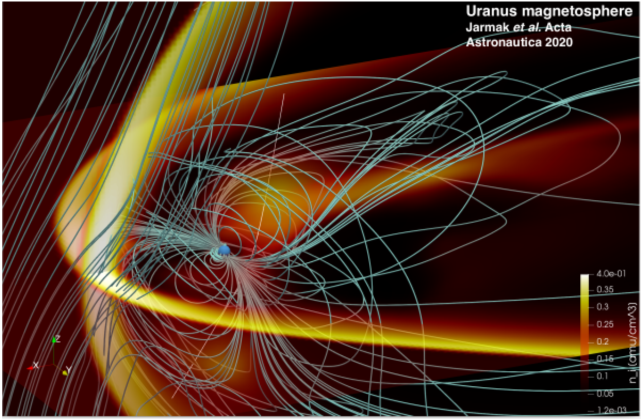



Figure: Ten-Moment simulation of Uranus's magnetosphere shows extremely complex magnetic-field structure due to dipole axis tilt with respective to revolution plane.

# Simple harmonic oscillator

Consider first the simple harmonic oscillator

$$\frac{d^2z}{dt^2} = \omega^2 z$$

This has exact solution $z = a\cos(\omega t) + b\sin(\omega t)$, where $a$ and $b$ are arbitrary constants. How to solve this numerically? Write as a system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = \omega^2 z$$

Note that the coordinates $(z, v)$ label the *phase-space* of the harmonic oscillator. Multiply the second equation by $v$ and use the first equation to get

$$\frac{d}{dt}\left(\frac{1}{2}v^2 + \frac{1}{2}\omega^2 z^2\right) = 0.$$

This is the *energy* and is *conserved*.
**Question: how to solve the ODE such that the energy is conserved by the discrete scheme?**

# Harmonic oscillator: Forward Euler Scheme

First attempt: use the simplest possible scheme, replace derivatives with difference approximations

$$\frac{z^{n+1} \quad z^n}{t} = v^n; \quad \frac{v^{n+1} \quad v^n}{t} = \quad \omega^2 z^n$$

or

$$z^{n+1} = z^n + \quad t v^n; \quad v^{n+1} = v^n \qquad t\omega^2 z^n$$

This is the *forward Euler* scheme. Lets check if the discrete scheme conserves energy:

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (1 + \omega^2 \quad t^2)((v^n)^2 + \omega^2 (z^n)^2)$$

The presence of the $\omega^2 \quad t^2$ in the bracket spoils the conservation. So the forward Euler scheme *does not* conserve energy. Also, note that the energy, in fact, is *increasing*!

# Harmonic oscillator: Forward Euler Scheme

Closer look: write as a matrix equation

$$\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & t \\ \omega^2 \quad t & 1 \end{bmatrix}}_{\text{acobian} \quad J} \begin{bmatrix} z^{n} \\ v^{n} \end{bmatrix}.$$

Observe that the determinant of the Jacobian is $\det(J) = (1 + \omega^2 \quad t^2)$ which is the same factor as appears in the energy relation. One may reasonably conjecture that when this determinant is one, then perhaps energy is conserved.

## Volume Preserving Scheme

We will call say a scheme preserves *phase-space* volume if the determinant of the Jacobian is $\det(J) = 1$.

# Harmonic oscillator: Mid-point Scheme

Perhaps a better approximation will be obtained if we use *averaged* values of $z, v$ on the RHS of the discrete equation:

$$\frac{z^{n+1} \quad z^n}{t} = \frac{v^n + v^{n+1}}{2}$$
$$\frac{v^{n+1} \quad v^n}{t} = \quad \omega^2 \frac{z^n + z^{n+1}}{2}$$

This is an *implicit* method as the solution at the next time-step depends on the old as well as the next time-step values. In this simple case we can explicitly write the update in a matrix form as

$$\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \frac{1}{1 + \omega^2 \quad t^2/4} \begin{bmatrix} 1 \quad \omega^2 \quad t^2/4 & t \\ \omega^2 \quad t & 1 \quad \omega^2 \quad t^2/4 \end{bmatrix} \begin{bmatrix} z^n \\ v^n \end{bmatrix}.$$

For this scheme $\det(J) = 1$. So the mid-point scheme conserves phase-space volume! Some algebra also shows that

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2$$

showing that energy is also conserved by the mid-point scheme.

# Harmonic oscillator: Mid-point Scheme is symplectic

A more stringent constraint on a scheme for the simple harmonic oscillator is that it be *symplectic*. To check if a scheme is symplectic one checks to see if

$$J^T \sigma J = \sigma$$

where $\sigma$ is the *unit symplectic matrix*

$$\sigma = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Turns out that the mid-point scheme for the harmonic oscillator is also symplectic. Note that if a scheme conserves phase-space volume, it *need not* be symplectic.

# Accuracy and Stability

To study the stability, accuracy and convergence of a scheme one usually looks at the first order ODE

$$\frac{dz}{dt} = \quad z$$

where $\quad = \lambda + i\omega$ is the complex frequency. The exact solution to this equation is $z(t) = z_0 e^{\quad t}$. The solution has damped/growing modes ($\lambda > 0$ or $\lambda < 0$) as well as oscillating modes.

- The forward Euler scheme for this equation is

$$z^{n+1} = z^n \qquad t \; z^n = (1 \qquad t \;)z^n.$$

- The mid-point scheme for this equation is

$$z^{n+1} = \left( \frac{1 \qquad t/2}{1 + \qquad t/2} \right) z^n$$

## Accuracy and Stability

We can determine how *accurate* the scheme is by looking at how many terms the scheme matches the Taylor series expansion of the exact solution:

$$z(t^{n+1}) = z(t^n)\left(1 \qquad t + \frac{1}{2} \;^2 \;\; t^2 \quad \frac{1}{6} \;^3 \;\; t^3 + \dots\right)$$

- The forward Euler scheme matches the *rst two terms*

$$z^{n+1} = z^n(1 \qquad t \;\;)$$

- The mid-point scheme matches the *rst three terms*

$$z^{n+1} = z^n\left(1 \qquad t \qquad \frac{1}{2} \;^2 \;\; t^2 \quad \frac{1}{4} \;^3 \;\; t^3 + \dots\right)$$

# Accuracy and Stability

We can determine if the scheme is *stable* by looking at the amplification factor $|z^{n+1}/z^n|$. Note that for damped modes ($\lambda > 0$) this quantity *decays* in time, while for purely oscillating modes ($\lambda = 0$) this quantity remains *constant*.

- The amplification factor for the forward Euler scheme in the absence of damping is $1 + \omega^2 \quad t^2 > 1$, hence this scheme is *unconditionally unstable*.
- The amplification factor for the mid-point scheme in the absence of damping is exactly 1, showing that the mid-point scheme is *unconditionally stable*, that is, one can take as large time-step one wants without the scheme "blowing up". Of course, the errors will increase with larger $\quad t$.

# Runge-Kutta schemes

- Even though the forward Euler scheme is unconditionally unstable, we can use it to construct other schemes that *are* stable and are also more accurate (than first order).
- For example, a class of Runge-Kutta schemes can be written as a combination of forward Euler updates. In particular, the *strong stability preserving* schemes are important when solving hyperbolic equations. Note that these RK schemes will *not* conserve energy for the harmonic oscillator, but *decay* it.
- Other multi-stage Runge-Kutta schemes can be constructed that allow very large time-steps for diffusive processes, for example, that come about when time-stepping diffusion equations.

## Simple harmonic oscillator

We looked at

$$\frac{d^2 z}{dt^2} = \quad \omega^2 z$$

and wrote it as system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = \quad \omega^2 z$$

Now introduce energy-angle coordinates

$$\omega z = E \sin\theta; \quad v = E \cos\theta$$

then $E^2 = \omega^2 z^2 + v^2 \equiv E_0^2$ is a constant as we showed before. Using these expressions we get the very simple ODE $\dot{\theta} = \omega$. This shows that in phase-space $(v, \omega z)$ the motion is with uniform angular speed along a circle.

# Simple harmonic oscillator: Phase-errors

The mid-point scheme had

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2 = E_0^2$$

which means that the mid-point scheme gets the energy coordinate *exactly* correct. However, we have

$$\tan \theta^{n+1} = \frac{\omega z^{n+1}}{v^{n+1}}.$$

Using the expressions for the scheme and Taylor expanding in $\quad t$ we get

$$\tan \theta^{n+1} = \tan \theta^n + \frac{\omega E_0^2}{(v^n)^2} \quad t + \frac{\omega^3 z^n E_0^2}{(v^n)^3} \quad t^2 + O( \quad t^3)$$

The first three terms match the Taylor expansion of the exact solution $\tan(\theta^n + \omega \quad t)$ and the last term is the *phase-error*.

# Single particle motion in an electromagnetic field

- In the Lagrangian frame the distribution function remains constants along *characteristics* in phase-space.
- These characteristics satisfy the ODE of particles moving under Lorentz force law

$$\frac{d\mathrm{x}}{dt} = \mathrm{v}$$
$$\frac{d\mathrm{v}}{dt} = \frac{q}{m}(\mathrm{E}(\mathrm{x}, t) + \mathrm{v} \times \mathrm{B}(\mathrm{x}, t))$$

- In the absence of an electric field, the kinetic energy must be conserved

$$\frac{1}{2}|\mathrm{v}|^2 = \text{constant}.$$

This is independent of the spatial or time dependence of the magnetic field. Geometrically this means that in the absence of an electric field the velocity vector rotates and its tip always lies on a sphere.

# Single particle motion in an electromagnetic field

- A mid-point scheme for this equation system would look like

$$\frac{\mathrm{x}^{n+1} \quad \mathrm{x}^n}{t} = \frac{\mathrm{v}^{n+1} + \mathrm{v}^n}{2}$$

$$\frac{\mathrm{v}^{n+1} \quad \mathrm{v}^n}{t} = \frac{q}{m} \ \overline{\mathrm{E}}(\mathrm{x}, t) + \frac{\mathrm{v}^{n+1} + \mathrm{v}^n}{2} \times \overline{\mathrm{B}}(\mathrm{x}, t))$$

  The overbars indicate some averaged electric and magnetic fields evaluated from the new and old positions. In general, this would make the scheme nonlinear!

- Instead, we will use a *staggered* scheme in which the position and velocity are staggered by half a time-step.

$$\frac{\mathrm{x}^{n+1} \quad \mathrm{x}^n}{t} = \mathrm{v}^{n+1/2}$$

$$\frac{\mathrm{v}^{n+1/2} \quad \mathrm{v}^{n \quad 1/2}}{t} = \frac{q}{m} \ \mathrm{E}(\mathrm{x}^n, t^n) + \frac{\mathrm{v}^{n+1/2} + \mathrm{v}^{n \quad 1/2}}{2} \times \mathrm{B}(\mathrm{x}^n, t^n))$$

# The Boris algorithm for the staggered scheme

The velocity update formula is

$$\frac{\mathrm{v}^{n+1\ \ 2} \qquad \mathrm{v}^{n\quad 1\ \ 2}}{t} = \frac{q}{m}\ \mathrm{E}(\mathrm{x}^n, t^n) + \frac{\mathrm{v}^{n+1\ \ 2} + \mathrm{v}^{n\quad 1\ \ 2}}{2} \times \mathrm{B}(\mathrm{x}^n, t^n))$$

This appears like an implicit method: most obvious is to construct a linear $3 \times 3$ system of equations and invert them to determine $\mathrm{v}^{n+1}$. Puzzle to test your vector-identity foo: find A if $\mathrm{A} = \mathrm{R} + \mathrm{A} \times \mathrm{B}$.

The Boris algorithm updates this equation in three steps:

$$\mathrm{v} \quad = \mathrm{v}^{n\quad 1\ \ 2} + \frac{q}{m}\mathrm{E}^n \frac{t}{2}$$

$$\frac{\mathrm{v}^{+} \qquad \mathrm{v}}{t} = \frac{q}{2m}(\mathrm{v}^{+} + \mathrm{v} \quad ) \times \mathrm{B}^n$$

$$\mathrm{v}^{n+1\ \ 2} = \mathrm{v}^{+} + \frac{q}{m}\mathrm{E}^n \frac{t}{2}$$

Convince yourself that this is indeed equivalent to the staggered expression above. So we have two electric field updates with half time-steps and a rotation due to the magnetic field. Once the updated velocity is computed, we can trivially compute the updated positions.

# The Boris algorithm for the staggered scheme

How to do the rotation? The Boris algorithm does this in several steps:

- Compute the t and s vectors as follows

$$\mathrm{t} = \tan\left(\frac{qB}{m}\frac{t}{2}\right)\frac{\mathrm{B}}{B} \approx \frac{q\mathrm{B}}{m}\frac{t}{2}$$

$$\mathrm{s} = \frac{2\mathrm{t}}{1+|\mathrm{t}|^2}$$

- Compute $\mathrm{v}' = \mathrm{v} \quad + \mathrm{v} \quad \times \mathrm{t}$ and finally $\mathrm{v}^+ = \mathrm{v} \quad + \mathrm{v}' \times \mathrm{s}$.

See Birdsall and Langdon text book Section 4-3 and 4-4 and figure 4-4a. Easily extended to relativistic case. Note that using the approxiate form in computing t will lead to *an error in the gyroangle*.

Note that in the absence of an electric field the Boris algorithm conserves kinetic energy.

# Why is the Boris algorithm so good?

See paper by Qin at. al. Phys. Plasmas, **20**, 084503 (2013) in which it is shown that the Boris algorithm *conserves phase-space volume*. However, they also show that the Boris algorithm is *not* symplectic.

- The relativistic Boris algorithm does not properly compute the $\mathrm{E} \times \mathrm{B}$ velocity. This can be corrected. For example Vay, Phys. Plasmas, **15**, 056701 (2008). The Vay algorithm however, breaks the phase-space volume preserving property of the Boris algorithm.
- Higuera and Cary, Phys. Plasmas, **24**, 052104 (2017) showed how to compute the correct $\mathrm{E} \times \mathrm{B}$ drift velocity and restore volume preserving property. Seems this is probably the current-best algorithm for updating Lorentz equations.
- The saga for better particle push algorithms is not over! For example, an active area of research is to discover good algorithms for *asymptotic* systems, for example, when gyroradius is much smaller than gradient length-scales or gyrofrequency is much higher than other time-scales in the system. Common in most magnetized plasmas.

# The Physics of Discretized Equations

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One view of computational physics: we are studying the *physics of discretized equations* and not really "Nature" itself. Not obvious that these are the same (as measure by some metric).

Many important physical properties are "indirect". Simplest example:

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

From this we can derive a conservation law for $L_2$ norm:

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

This is an example of an "indirect" property. **Not obvious** that the $L_2$ norm of your discrete solution is actually preserved by the scheme you choose. In fact, **not obvious** if it even *should* be preserved!

# The Physics of Discretized Maxwell Equations

Maxwell equations have very important *indirect* properties: conservation of momentum and energy. Energy conservation is the $L_2$ norm of the field:

$$\frac{\partial}{\partial t}\left(\frac{\mathbf{B}^2}{2\mu_0} + \frac{\epsilon_0 \mathbf{E}^2}{2}\right) + \frac{1}{\mu_0}\nabla\cdot(\mathbf{E}\times\mathbf{B}) = \quad \mathbf{E}\cdot\mathbf{J}.$$

- Does a scheme conserve the *discrete* energy? *Should* it conserve discrete energy?
- Choices based on tradeoff one is willing to make.

# E ect of Discrete Energy Conservation

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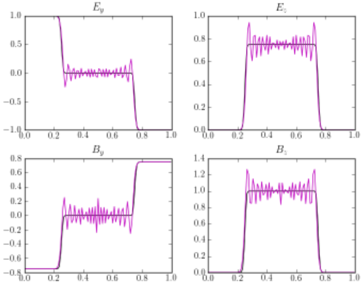


Figure: Energy conserving scheme for Maxwell equations (purple) compared to exact solution (black). Conservation of energy means there is no damping of spurious high-$k$ modes.

# Energy Conservation in Vlasov-Maxwell is Indirect

If we evolve the Vlasov equation we are evolving the distribution function $f(\mathrm{x}, \mathrm{v}, t)$ in phase-space. However, total energy is a *moment* of the distribution function and also includes electromagnetic terms.

$$\frac{d}{dt}\sum_s \int_K \frac{1}{2} m|\mathrm{v}|^2 f \, dz + \frac{d}{dt}\int \left( \frac{\epsilon_0}{2}|\mathrm{E}|^2 + \frac{1}{2\mu_0}|\mathrm{B}|^2 \right) d^3\mathrm{x} = 0$$

Not obvious that a scheme will conserve total energy.

# Energy Conservation in Hamiltonian Systems

Many plasma problems are described by Hamiltonian system of equation: Vlasov-Poisson equations, gyrokinetic equations, several ideal fluid models.

$$\frac{\partial f}{\partial t} + \{f, H\} = 0$$

where $\{f, g\}$ is a Poisson-bracket operator and $H$ is a Hamiltonian. Example of Vlasov-Poisson equations:

$$H(\mathrm{x}, \mathrm{v}) = \frac{1}{2} m v^2 + q\phi(\mathrm{x})$$

with the bracket

$$\{f, g\} = \frac{1}{m} \; \nabla_{\mathrm{x}} f \cdot \nabla_{\mathrm{v}} g \quad\;\; \nabla_{\mathrm{x}} g \cdot \nabla_{\mathrm{v}} f \Big) + \frac{q\mathrm{B}_0}{m^2} \cdot \nabla_{\mathrm{v}} f \times \nabla_{\mathrm{v}} g$$

# Energy Conservation in Hamiltonian Systems

- Energy conservation in Hamiltonian systems are also indirect. These follow from the property of the Poisson-bracket that

$$\int_K f\{f,H\}\,dz = \int_K H\{f,H\}\,dz = 0.$$

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- It is not obvious that a scheme will preserve these property: former is required for entropy conservation, and the latter for energy conservation
- Worse, there is no guarantee that the distribution function remains positive! Very serious problem.
- Adjusting the distribution function via simple positivity fixes can add huge energy conservation errors for many problems.

# The Question of Discrete Entropy

In addition to momentum and energy, the Vlasov-Maxwell and other equations have an entropy that is either constant (collisionless plasma) or increases monotonically (collisional plasmas)

$$\frac{d}{dt}\int_K f\ln(f) \geq 0.$$

Again, it is not immediately clear how the entropy of the discrete system behaves. Connected to the behavior of $f^2$ and positivity of $f$.

## A More Subtle Form of Indirect Properties

Even if you *have* an explicit conservation law, there are other subtle properties that are indirect. For example, typical fluid codes will evolve total energy equation

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot [\mathrm{u}(\mathcal{E} + p)] = 0.$$

where total energy $\mathcal{E}$ contains two contributions, one from the kinetic energy and the other from the internal energy:

$$\mathcal{E} = \frac{1}{2}\rho \mathrm{u} \cdot \mathrm{u} + \frac{p}{\quad 1}$$

# The Behavior of Kinetic Energy

Now consider the evolution of just the *kinetic energy*

$$\frac{\partial}{\partial t}\int \frac{1}{2}\rho u^2 \, d\mathrm{x} + \oint_{\partial} \left(\frac{1}{2}\rho u^2 + p\right) \mathrm{u}\cdot \, d\mathrm{s} \qquad \int p\nabla\cdot \mathrm{u} \, d\mathrm{x} = 0.$$

- This equation shows that the KE in a volume only changes due to the compressibility of the fluid.
- Similarly, in a plasma, there will be $\mathrm{J}\cdot\mathrm{E}$ term that allows energy exchange between particles and fields.

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An incorrect discrete exchange can lead to improper behavior of energy at the highest-$k$ modes. These modes are precisely what we need to get correct to understand turbulence!

# What Does All This Mean?

- Many of the indirect properties listed above are required for robust and physically correct simulations: not enough to focus only on convergence and stability of the scheme!
- Often one must make a trade off: there is no "free lunch" and depending on the problem one must choose what property to pursue.

# Consider the Advection Equation

To fix ideas consider we wish to solve the advection equation

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

Using the four-cell symmetric recovery scheme to compute interface values in the FV update formula we get the semi-discrete scheme *ve-cell stencil* update formula:

$$\frac{\partial f_j}{\partial t} = \quad \frac{1}{\ x} \int_{x_{j\ \ 1\ 2}}^{x_{j+1\ 2}} \frac{\partial f}{\partial x}\, dx = \quad \frac{1}{12\ \ x}(f_{j\ \ 2} \quad 8 f_{j\ \ 1} + 8 f_{j+1} \quad f_{j+2})$$

This scheme conserves $L_2$ norm! How accurate is this scheme, or what is its order of convergence? Does this scheme maintain monotonicity and positivity?

# Advection Equation: Central 4th Order Scheme

Central 4th order scheme (conserves $L_2$ norm)

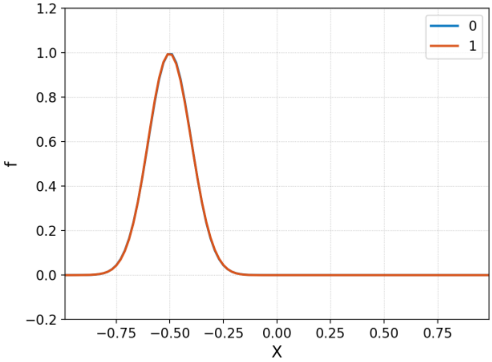


Figure: Blue: Exact solution. Orange: Central 4th order solution

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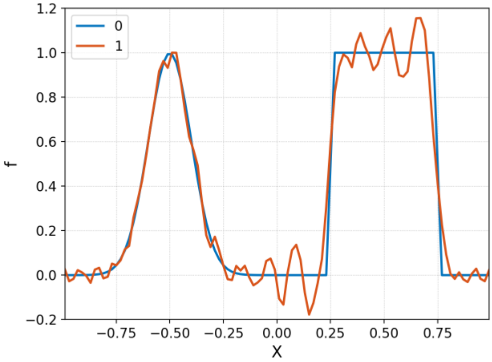


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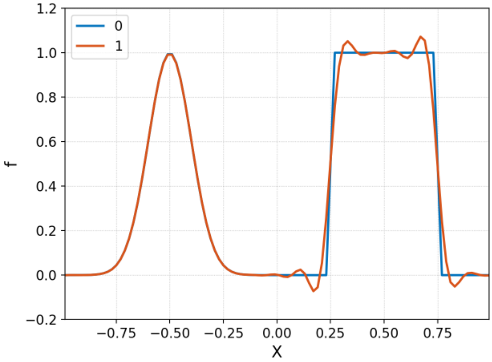
# Advection Equation: Upwind 5th Order Scheme

Upwind 5th order scheme (*does not* conserves $L_2$ norm)

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# Godunov's Theorem

- A very important theorem proved by Godunov is that there is **no** *linear scheme* that is "monotonicity preserving" (no new maxima/minima created) and **higher than rst-order accurate**!

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- A very important theorem proved by Godunov is that there is **no** *linear scheme* that is "monotonicity preserving" (no new maxima/minima created) and **higher than rst-order accurate**!
- Consider a general scheme for advection equation

$$f_j^{n+1} = \sum_k c_k f_{j+k}^n.$$

The discrete slope then is

$$f_{j+1}^{n+1} \quad f_j^{n+1} = \sum_k c_k \quad f_{j+k+1}^n \quad f_{j+k}^n \big) .$$

Assume that all $f_{j+1}^n \quad f_j^n > 0$. To maintain monotonicity at next time-step hence one must have all $c_k \geq 0$.

# Godunov's Theorem

- First order upwind scheme:

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{\Delta x}(f_j^n - f_{j-1}^n)$$

this satisfies monotonicity as long as $\Delta t/\Delta x \leq 1$.

- Second order symmetric scheme

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{2\Delta x}(f_{j+1}^n - f_{j-1}^n)$$

clearly this does not satisfy the condition of monotonicity.

- In general, condition on Taylor series to ensure atleast second-order accuracy shows that at least *one* of the $c_k$s must be negative. Hence, by contradiction, *no such scheme exists*!

# Godunov's Theorem: Consequences and Workarounds

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- However, Godunov's theorem shows that this "diffusion" must be dependent on the local solution itself and can't be fixed *a priori*. This means a **monotonicity preserving scheme must be nonlinear**, even for linear hyperbolic equations.
- Leads to the concept of *limiters* or artificial viscosity, that control the monotonicity violations (adding diffusion to high-$k$ modes). No free lunch: limiters must diffuse high-$k$ modes but this will inevitably lead to issues like inability to capture, for example, high-$k$ turbulence spectra correctly without huge grids.
- Major research project: interaction of shocks, boundary layers and turbulence in high-Reynolds number flows.

# The FV Revolution in computational fluid dynamics

In the mid and late 20th century a major revolution occurred in solution of hyperbolic PDEs

- Driven by need to solve Euler and Navier-Stokes equations for airplanes, the space-program and other problems
- Even a subsonic jet (Mach 0.8) can have local pockets of supersonic flow. Reentry vehicles develop bow shocks as they enter the atmosphere
- The idea to use *nonline r* schemes occurred to many people. Including von Neumann and Ritchmyer (1950).
- Key breakthrough was discovery of MUSCL scheme by van Leer. "Towards the Ultimate Conservative Difference Scheme" (1970s). Part V has $> 5000$ citations. Extremely impactful.
- Discovery of many schemes, ENO, WENO, PPM, Wave-Propagation, MP. Massive research in limiters
- Driven in large part by few people: van Leer, Ami Harten, Phil Roe, Phil Collela, Randy LeVeque, Marsha Berger, Stan Osher, Tony Jameson, Chi-Wang Shu, Peter Lax, ...

# Nonlinear flux limiters: Getting around Godunov

To get around Godunov's Theorem we need to construct a *nonlinear scheme*, even for linear equations. One apporach is to use nonlinear flux-limiters:

$$F_{j+1/2} = \phi(r_{j+1})F_{j+1/2} + \;\; 1 \quad \phi(r_{j+1})\big)F^{L}_{j+1/2}$$

where $\phi(r) > 0$ is a *limiter* function: chooses between *high-order* and *low-order* flux.

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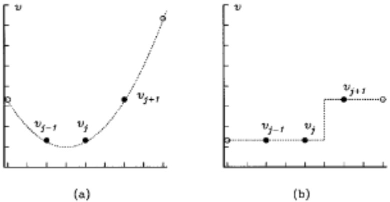
The first-order upwind flux is "Total-Variation Diminishing" (TVD), $\mathrm{V}(f^{n+1}) \leq \quad \mathrm{V}(f^{n})$ where "Total-Variation" is defined as:

$$\mathrm{V}(f) = \sum_j |f_{j+1} \quad f_j|$$

# Nonlinear flux limiters: No “Perfect” Limiter!

- Unfortunately, there is no perfect limiter (though some come close to perfection): depends on problem and best to implement many!
- Most limiters “chop off” genuine maxima/minima: notice that $\phi(r < 0) = 0$ which means that if there is a genuine maxima/minima then low-order flux is selected.
- Tricky to distinguish step-function from parabola!
  Accuracy-preserving limiter: Suresh and Huynh, JCP **136**, 83-99 (1997). Not an easy paper to understand.



# Advection Equation: Monotone 5th Order Scheme

Monotone, upwind 5th order scheme (*does not* conserves $L_2$ norm)