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Computational Methods I)

Join the GitHub → first via slides on GSS website.

Goal: Modern Computational Techniques for PP.

PP uses Vlasov - Maxwell Eqns

$$\frac{\partial f_s}{\partial t} + \nabla_{\vec{x}} \cdot (\vec{v} f_s) + \nabla_{\vec{v}} \cdot (F_s f_s) = \left(\frac{\partial f_c}{\partial t}\right)_c \nearrow \text{collision terms.}$$

Describe self-consistent evolution of distribution function $f(\vec{x}, \vec{v}, t)$ and electromagnetic fields.

$\vec{F}_s \equiv$ Lorentz force.

This equations are highly nonlinear => Highly difficult to solve Vlasov-Maxwell eqn

Because of difficulty, we have many approximations to simplify greatly.

Approximations)

- Discovery of gyrokinetic equations → asymptotic approx for plasmas in strong magnetic fields. Fast frequencies can be neglected, increasing simplicity.

- Fluid approximations => MHD (but lose kinetic effects).

- Computational physics can be an application tool, or as an area of legitimate research area.
  (In situ => In space)

→ The EM fields are determined by Maxwell's equations.

Conservation properties are in Vlasov - Maxwell Eqns:

- Conserves particle number
- Conserves Total (particle + field) momentum
- Conserves Total (particle + field) energy.

Ammar Hakem, very eloquent, [redacted].

Computational Physics II)

Single Particle Motion in an EM Field)

First, SHO) $\frac{d^2 z}{dt} = -\omega^2 z \Rightarrow z = a\cos(\omega t) + b\sin(\omega t)$

Solve numerically first $\Rightarrow$ $\frac{dz}{dt} = v$, $\frac{dv}{dt} = -\omega^2 z$, note (z, v) label the phase space of HO.

$$\frac{d}{dt}\left(\frac{1}{2}v^2 + \frac{1}{2}\omega^2 z^2\right) = 0 \Rightarrow \text{Energy, and is conserved}$$

Numerically, can replace derivatives by finite differences.
(Forward Euler Scheme)

$$\frac{z^{n+1} - z^n}{\Delta t} = v^n, \quad \frac{v^{n+1} - v^n}{\Delta t} = -\omega^2 z^n$$; this, if extrapolated

out, we see that energy is not conserved, energy increases.

Numerical methods of solving the SHO eqn, even if the energy is conserved (mid pt. scheme), we still had phase errors in those graphs, getting worse in time.

Stability is good if det (Jacobian) of amplification factor.

Runge-Kutta Scheme $\rightarrow$ Constructed from forward Euler Scheme.
- even though Forward Euler scheme is unconditionally unstable, we can use multiple "bits" or "scheme" to get a more accurate, agreeable

Motion in EM Field) Even if E, B given, we can't use the midpoint scheme, b/c we get averages of E, B, which we're not given.
- Use a staggered scheme!

Boris Algorithm)

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Computational Methods II)

Boris Algorithm)

- Boris algorithm exactly conserves energy for single motion in EM field
- It is also volume conserving scheme (det(Jacobian) = 1)
  + Deals w/ conservation of phase space volume.

Current best => $\boxed{\text{Higuera + Cary}}$ for relativistic single particle motion in EM field. Preserves conservation of phase space that Boris got for nonrelativistic effect, and correctly accounts for E×B velocity in relativistic regime.

Vlasov Equation removes all single particle effects, so no radiative effects are accounted for in Vlasov; you'd have to account for that seperately.

• Debye shielding does not exist in gravitational systems, like galactic dynamics, globular clusters, self-gravitating system.
- kinetic theory is used in plasmas, now being used in gravitational astrophysics and gaxay theory

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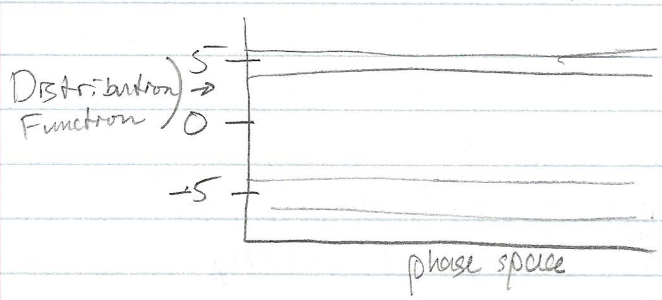
Looking to solve Vlasov-Maxwell equations.

Simulation → Classic 2 stream instability



=> Forms "BGK" modes w/ small perturbation.

Classical Helmholz - kelvin instabilities, super super cool simulation, has all 3 ranges, w/in the simulations.

Computational Physics III)

Recall scheme conserves volume phase space if det(Jacobian) = 1
- Midpoint scheme conserves energy.

Particle in motion in conservative force for given $\phi(x)$

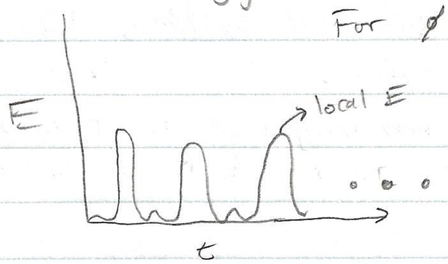
$$W = \frac{1}{2}v^2 + \phi = \text{constant}, \quad \text{for } \frac{dx}{dt} = v, \quad \frac{dv}{dt} = -\frac{\partial \phi}{\partial x}$$

Implicit methods won't work, need iterative process.

Look @ Boris (staggered timestep), for conservative force:
- Is energy conserved?

In the staggered method, energy oscillates about some mean method

For $\phi = \sin x$



⊛ Define some quantity that will actually be conserved, even though E oscillates.

Ask) How do you know what quantity to define that yields a conservative result?

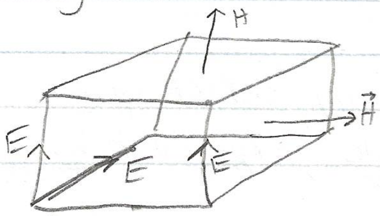
Solving Maxwell Eqns) There are global conservation laws
- How can we actually solve M.E. efficiently and maintain (some) conservation + geometric properties?

- The M.E. geometry doesn't readily come out from compact form.

$\vec{E}$ is a vector, while $\vec{B}$ is a bivector
↳ They are different, so solving M.E. must treat E, B differently.

(Computational Physics III)

Solving M.E. => The Yee-cell.



Electric field should be on edges, while Mag field is a bivector, should be on faces

- This can also be flipped => evidence of Duality of E + B fields.

• In spacetime, EM fields => $F_{\mu\nu}$, bivector.

stagger them, by 1/2 step

Now calculate 2 curls $\frac{\partial B}{\partial t} + \nabla \times E = 0$, $\epsilon_0 \mu_0 \frac{\partial E}{\partial t} - \nabla \times \vec{B} = 0$,

Define two different grad operators, ∇_E, ∇_F, one on edges, other on faces.

The curl operator ∇_E takes stuff on edges, moves to faces.
" " ∇_F " " " faces, moves to edges!

What if we reintroduce currents? -> Geometry must be conserved; so current must be a vector, needs to be on the edges!,

• Staggering in time reflects that in 4D, EM field is a bivector in spacetime.

=> staggering also applies to Dirac equations, can solve them.

Divergence in Yee-cell.

$$\left.\begin{aligned} \nabla_F \cdot \vec{B}^{\,n+1/2} &= 0 \\ \nabla_E \cdot \vec{E}^{\,n} &= 0 \end{aligned}\right\} \text{ Exactly maintained w/ the Yee-mesh.}$$

For plasma, we have current conservation: $\frac{\partial \rho_c}{\partial t} + \nabla \cdot \vec{J} = 0$,
on Yee-cell:

$$\frac{\rho_c^{\,n+1} - \rho_c^{\,n}}{\Delta t} + \nabla_E \vec{J}^{\,n+1/2} = 0$$

Computational Physics III)

Maxwells eqns are hyperbolic

- Small disturbance in system described by set of eqns. If the speed @ which disturbance travels is finite, eqns are hyperbolic
  ↳ speed of light for EM.

Consider $\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial t} = 0$, $\vec{F} = \vec{F}(\vec{Q})$

Compute flux - Jacobian $A = \frac{\partial \vec{F}}{\partial \vec{Q}}$. Calculate eigenvalues/vectors. If real, and complete

If $\vec{A}$ is diagonalizable, they are hyperbolic equations.

Consider $\frac{\partial}{\partial t}\begin{bmatrix} E_y \\ B_z \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} c^2 B_z \\ E_y \end{bmatrix} = 0$,

Flux-Jacobian $A = \begin{bmatrix} 0 & c^2 \\ 1 & 0 \end{bmatrix}$

Values : $r' = \begin{bmatrix} 1 \\ -1/c \end{bmatrix}$ → real, and yields max speed @ which disturbance propagates

Consider ideal fluid eqns. (Euler Eqns) => They're hyperbolic

3 eigenvalues : velocity of fluid, $u \pm C_s$, where $C_s \equiv$ sound speed.
=> Hyperbolic, but nonlinear hyperbolic.

Other examples => ideal MHD eqns, relativistic fluid eqns, Einstein field eqns.

If flux-Jacobian, and eigenvalues are found, values give all speeds w/in system => Alfvèn speed, slow MD speed, other characteristics we should be familiar with.

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Computational Physics III)

Hyperbolic problems require very special methods to solve!
- major features of H.E.'s exhibit shocks, rarefactions, contact discontinuities, etc.)

· Looked into shock capturing methods.
- developed to ~~a~~ simulate aerospace engineering (supersonic flight, transonic flight, re-entry into atmosphere)

NY → Paris in 90 mins ⟹ Mach 5, hypersonic flight.
Fusion physics, shock capturing methods aren't widely used, but Astrophys plasmas widely use shock capturing methods.
- apparently fusion machine plasma evolution is too slow to justify shock capturing methods.

· Are Vlasov eqns hyperbolic? ⟹ yes, but only finite dimensionally.

IV

Galerkin scheme. Discontinuous ⟹ solution represented using piecewise discontinuous functions. ⟹ solving hyperbolic PDE

→ DG

- need Galerkin minimization,
→ state of the art currently.

· First introduced in 1973, as conference paper to solve steady state neutron transport in reactors. → linear system.
- 25 yrs. later first application of DG in nonlinear systems.

Example) L_2 minimization of errors on finite dimensional set
Legendre Polynomials. Interval $[-1, 1]$

$$(f, g) = \int_{-1}^{1} f(x) g(x)\, dx$$

Select inner product, use to define norm.
Consider time-dependent problem on $x \in [-1, 1]$

$$f(x,t) \approx f_h(x,t) = \sum_{k=1}^{N} f_k(t) P_k(x) \quad \text{yields} \quad \sum f_k' P_k(x) = G[f_h]$$

⟹

$$\|L\|_2 = (f,f)$$

Computational Physics IV)

Now we want to find the f'_k Error function $\Rightarrow$ L_2 norm

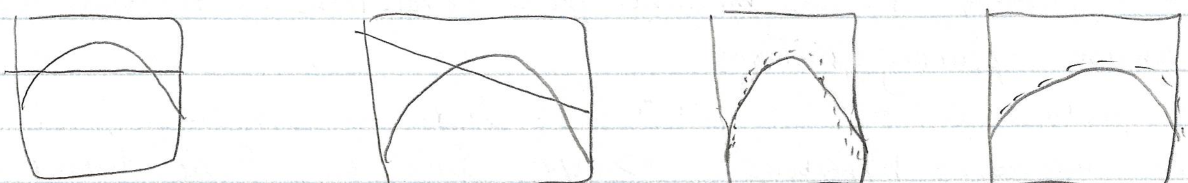
$$E_N = \left\| \sum f'_k P_k(x) - G[f_h] \right\|_2 = \int_{-1}^{1} \left[\sum f'_k P_k(x) - G[f_h] \right]^2 dx$$

Find minimum: $\frac{\partial E_N}{\partial f_m} = 0$ for all $k = 1, 2, \ldots, N$.

Gives a set of equations that minimize error in our problem.

Consider finding best fit on finite-dimensional space for

$$f(x) = 3 + (x - 0.5)^4 + 2x^3 - 5x^2 \quad \text{on } x \in [-1, 1]$$



P_1 $\qquad$ P_1, P_2 $\qquad$ P_1, P_2, P_3 $\qquad$ exact P_4

Highest polynom. in $f(x)$ is 4, so gives exact fit when using P_4

- These are the piecewise functions ↑

DG, split intervals into cells and use Galerkin scheme in each cell.
- Note the discontinuous lines are representations of our solution, keep in mind.

So we can relate representation w/ solution Use weak-equality

Definition. Weak Equality.

2 fxns, f, g are weakly equal if

$$(\psi_k, f - g) = 0 \quad \text{for all } k = 1, \ldots, N$$

Then $f \doteq g$

Computational Physics IV

We relate LHS, RHS via weak equality $f'(x,t) \doteq G[f]$, this implies

$$(\psi_k,\ f'(x,t) - G[f]) = 0$$

Consider a linear represen. of particle distribution fxn:

$f_h(x) = f_0 + x f_1$ in a cell. Reconstruct an exponential function to describe

This can be negative, not good. Exponentials make all > 0, so no negatives, good.

"Example of recovery: Exponential recovery in a cell".

DG scheme for linear advection
Consider 1D passive advective eqn on $I \in [L, R]$

$$\frac{\partial f}{\partial t} + \lambda \frac{\partial f}{\partial x} = 0, \quad \lambda \equiv \text{const. advective speed.}$$

Exact solution: $f(x,t) = f_0(x - \lambda t)$, for $f_0(x) \equiv IC$.

1) Discretize into elements

$$I_j \in [x_{j-1/2},\ x_{j+1/2}]$$

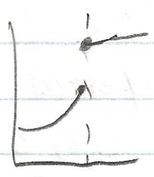
2) Pick finite dimensional basis to work from (Legendre, etc).

③ L_2 minimization
Find f_h in fxn space such that for basis fxn ϕ is

$$\int_{I_j} \phi \left(\frac{\partial f_h}{\partial t} + \lambda \frac{\partial f_h}{\partial x} \right) dx = 0$$

IBP to move derivative onto basis functions.

at discontinuous breaks, we have 2 values



which value to pick?

- Look and see how information is flowing, that will inform which value above to pick.

Computational Physics IV

Also, no choice is wrong; we can average, or just pick, etc.
But some choices yield better fits for the solution representation.
- Averages typically look better, but can go negative which isn't good.
- Choose upwinding value, and use higher order basis terms, and our fit looks quite good.

Does our scheme satisfy certain characteristics (like for continuous passive equation, do we get particle conservation from our representation?)
- The average value conserves particles, but is a bad representation
- The upwinding soln doesn't conserve particles but is good representation.
→ Need to look carefully at these things.

Now apply it to a problem ⇒ Putting everything together, Vlasov-Maxwell eqn using DG.

Treat Vlasov as PDE in (6D). How do we solve this and return invariance. (particles, total momentum, total energy)
- total energy is conserved, but momentum is not

Need to make sure entropy increases in your scheme.

Advice ⇒ Every day, read the plasma physics archive
arxiv physics.comp-ph and numerical analysis math.NA
and plasma archive

Learn C++!

Learn) expert@ (i) the physics, (ii) mathematics of the numerical methods, and (iii) program and software techniques
↳ Apparently these skills are in insanely high demand!