DL-GPU Workshop Day 5

Friday, July 28, 2023 9:46 AM

On the topic(s) of Computational Plasma Physics.

Governing equations & Normalization

Plasma:
- A group of charged particles.
- with collective behavior
- quasi - neutral

- λ_D vs L (spatial)

- ν_{pe} greek "\nu" vs. ν_{en} (temporal)
  → collision frequencies. microscopic.

High - fidelity / Physics - based.

Particle - kinetic modeling approach.

- Use a large number of "simulation particles" to emulate the physics of the system.

*) Single particle motion. (Lorentz).

Lorentz force Newton's 2nd Law

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) = m\vec{a} = m\frac{d\vec{v}}{dt}$$

F: force. q: charge; $\vec{E}$: electric field.

$\vec{v}$: particle velocity $\vec{B}$: B field
m: mass of particle. t: time

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Governing eqs & Normalization.

In particle simulations, often normalize:

Field eqn: (electrostatics)

$$-\nabla \cdot (\varepsilon \nabla \phi) = \rho_i - \rho_e$$

PDE: $\nabla \cdot (\varepsilon \cdot \nabla \phi) = \rho$

Poisson's Eq.

∇: gradient / divergence operator.

∇ $\nabla \cdot$

$\nabla \cdot (\varepsilon \cdot \nabla \phi) = 0$

Laplace Eq.

ρ: charge density i/e: ions / electrons.

ε: permittivity of medium (free space).

Why normalization?

Some physical constants are too large (10^{23} "mole") or too small (e.g., mass of an electron, 10^{-31} kg?) → "round-off" error in computer simulations.

To reduce the round-off error, we normalize the governing eqns., s.t.

$$\hat{a} = \frac{a}{a_{ref}}$$

a ← in physical unit

a_{ref} ← reference value, in physical unit.

$\hat{a}$ → dimensionless, "normalized".

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Let's start from a simple case. no B field. electrostatic problem.

Eqn of Motion: (E.O.M.)

$$\vec{F} = q\vec{E} = m\vec{a} = m\frac{d\vec{v}}{dt}$$

E field:

$$-\nabla\cdot(\varepsilon_0 \nabla\phi) = \rho_i - \rho_e$$

$$\vec{E} = -\nabla\phi.$$

ϕ: electric potential scalar.

Normalize:

$$\hat{q} = \frac{q}{q_{ref}}; \quad \hat{\vec{E}} = \frac{\vec{E}}{\vec{E}_{ref}}; \quad \hat{\vec{v}} = \frac{\vec{v}}{\vec{v}_{ref}},$$

$$\hat{t} = \frac{t}{t_{ref}};$$

Rewrite: $q = q_{ref}\cdot\hat{q}$; $\vec{E} = \vec{E}_{ref}\cdot\hat{\vec{E}}$; etc.

plug into the governing eqns:

plug in the ref. values.

$$\underbrace{q_{ref}}_{e}\hat{q}\cdot\vec{E}_{ref}\cdot\hat{\vec{E}} = \underbrace{m_{ref}}_{m_e}\hat{m}\cdot\frac{d\vec{v}_{ref}\cdot\hat{\vec{v}}}{dt_{ref}\cdot\hat{t}}$$

Q: How to choose "ref" values?

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If we choose: $q_{ref} = e$, elementary charge $\sim 1.6 \times 10^{-19}$ C.

Volt.

$$E_{ref} = \frac{\phi_{ref}}{L_{ref}} = \frac{\frac{kT_e}{e}}{L_{ref}} \quad \frac{kT_e}{e} \rightarrow \frac{[eV]}{e} \rightarrow [V]$$

$$L_{ref} = \lambda_D = \sqrt{\frac{\varepsilon_0 k T_e}{n_e \cdot e^2}}$$

$m_{ref} = m_e$. ele. mass.

$$V_{ref} = V_{te} = \sqrt{\frac{kT_e}{m_e}}$$

thermal velocity of ele.

kT_e : in $[eV] \rightarrow [J]$ energy Joules.

m : mass.

microscopic: atoms / molecules.

vel. of random motion.

$\frac{1}{2} m v^2 \sim [J]$

$$t_{ref} = \frac{1}{\omega_{pe}} = \sqrt{\frac{m_e \cdot \varepsilon_0}{n_e \cdot e^2}} \quad [s] \text{ SI units.}$$

Plug in:

$$e \hat{q} \cdot \frac{\frac{kT_e}{e}}{\sqrt{\frac{\varepsilon_0 kT_e}{n_e \cdot e^2}}} \cdot \hat{\vec{E}} = m_e \cdot \hat{m} \cdot \frac{\sqrt{\frac{kT_e}{m_e}} \cdot d\hat{\vec{v}}}{\sqrt{\frac{m_e \varepsilon_0}{n_e \cdot e^2}} \, d\hat{t}}$$

$$\hat{q} \cdot \hat{\vec{E}} = \hat{m} \cdot \frac{d\hat{\vec{v}}}{dt}$$

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$$\boxed{\hat{q} \cdot \hat{\vec{E}} = \hat{m} \cdot \frac{d\hat{\vec{v}}}{d\hat{t}}}$$

Same form as the version with physical units.

e.g.: physical unit / dimensional:

$$m_e = 9.1 \times 10^{-31} \text{ kg}$$

normalized / dimensionless.

$$\hat{m}_e = 1.$$

Big difference in numerical computing.

~ 1960's - 1970's

Similarly, for field eqn:

$$-\nabla \cdot (\varepsilon \nabla \phi) = \rho \implies \nabla \cdot (\varepsilon \nabla \phi) = -\rho$$

use: $\hat{\varepsilon} = \frac{\varepsilon}{\varepsilon_{ref}} = \frac{\varepsilon}{\varepsilon_0}$, $\hat{\rho} = \frac{\rho}{\rho_{ref}} = \frac{\rho}{n_e \cdot e}$ $\left(\frac{C}{m^3}\right)$

$$\hat{\phi} = \frac{\phi}{\phi_{ref}} = \frac{\phi}{kT_e/e}$$

differential operator: $\boxed{\nabla := \frac{\hat{\nabla}}{L_{ref}}}$

$$\nabla \sim \frac{\partial}{\partial x} = \frac{\partial}{\partial L_{ref} \cdot \hat{x}} = \frac{1}{L_{ref}} \frac{\partial}{\partial \hat{x}} = \frac{1}{L_{ref}} \cdot \hat{\nabla}$$

$\implies$ Plug into Poisson's eq.

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$$\Rightarrow \boxed{\hat{\nabla}\cdot(\hat{\varepsilon}\cdot\hat{\nabla}\cdot\hat{\phi}) = -\hat{\rho}}$$. Normalized field eqn.

Significance / Beauty of Normalization:

- same form of equations.
- Reduce numerical round-off error.

Lunch Break till 1:30 PM. Central.

11:30 AM. Pacific

Back from lunch break. ~1:34 PM. Central.

Overview of computational techniques in plasma physics. (kinetic)

- Overall, we have the approaches of ① Theory ② physical experiment. ③ Computer experiment. (Simulation)

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physical phenomena → Math Model(s).
(ODE's, PDE's)

↓

Discrete Approximation
(FD, FE, FV)

↓

Numerical Algorithms.
(pseudo-codes)

↓

Simulation Programs.
(Source codes, Fortran / C / C++
Java Py)

Computational techniques.

"software engineer" training.

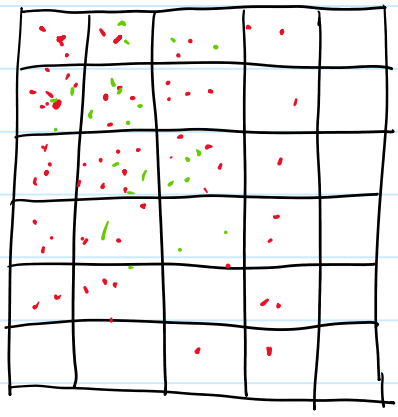
R&D. Academic.

(Code developer & user)

Computer experiment ← (simulations)

Kinetic modeling / simulation for plasma dynamics.

E.g. 2-D, electrostatic.



- Computation mesh Cartesian "cell"
- **Particles.** $(\vec{x}, \vec{v})$ continuous in phase space $(\vec{x}, \vec{v})$ 6-D.

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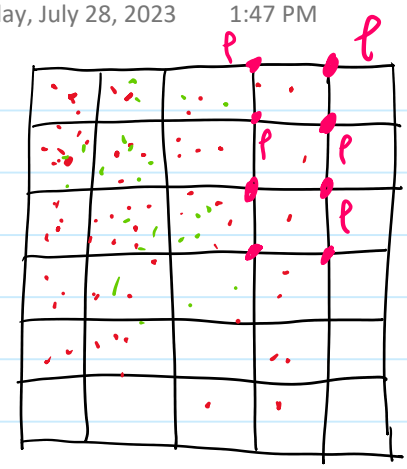


- Field quantities: n, ρ, ϕ, $\vec{E}$,

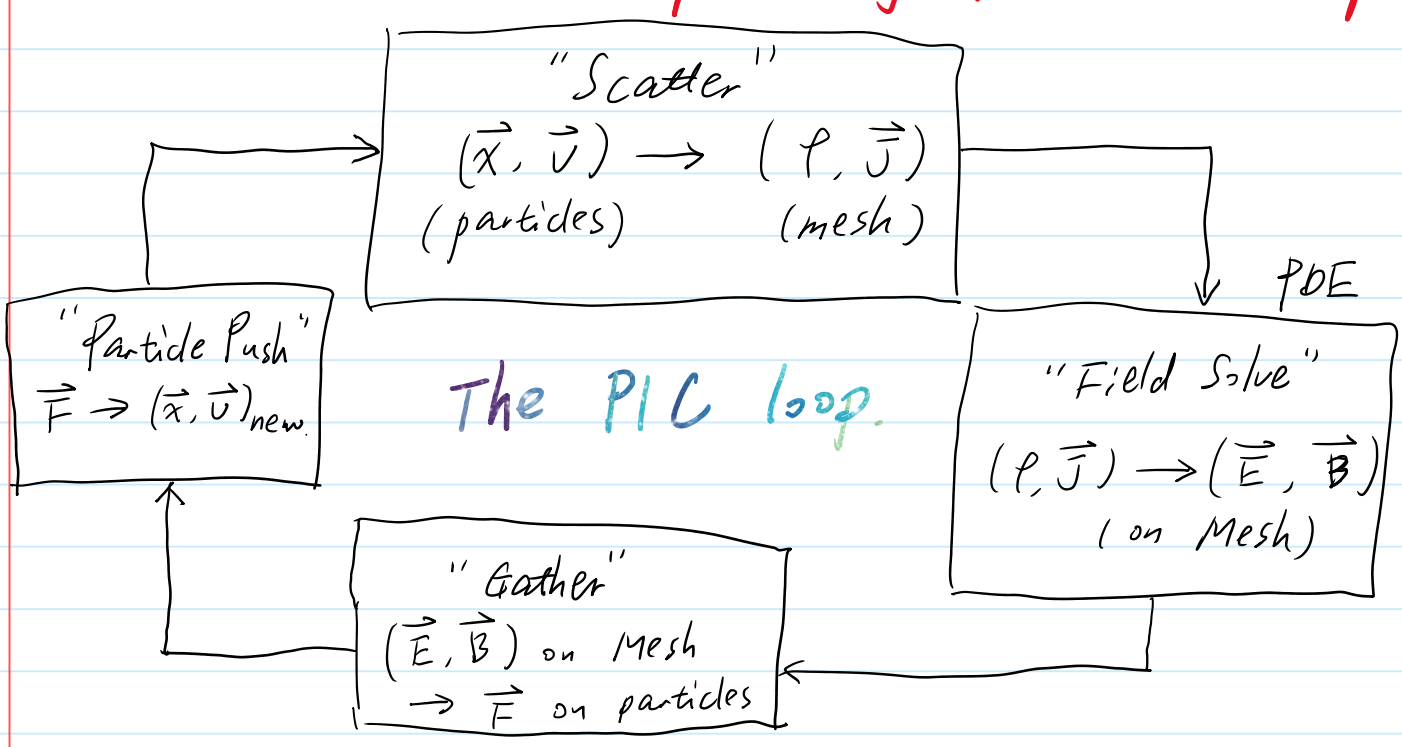
stored on discretized computation mesh. (nodes or faces / edges of each "cell").

Problem / Question: How to emulate / evolve the physical processes.

Rephrase: How to track motions of each particle?

"Particle-in-Cell": PIC.

The essential kernel part of PIC is a loop.



The PIC loop.

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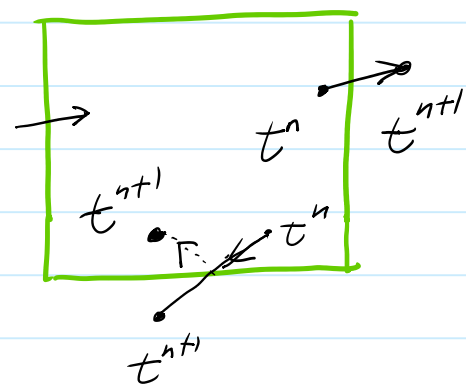
Steps in addition to the PIC Loop:

- Initialization. ("t=0"). - sample/load particles into the computation.

- BC. Boundary conditions: - Field. (PDE)

  - Particle.



Back at 2:40 PM Central

12:40 PM. Pacific.

Question: How to tell whether the simulation results are good or not?

$2+4=7$; $2+4=6$

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E.O.M: $q\vec{E} = \vec{F} = m\vec{a} = m\dfrac{d\vec{v}}{dt}$.

$$\begin{cases} \vec{v}^{new} = \underline{0.5}\,\vec{v}^{old} + \vec{a}^{old}\cdot\Delta t \\ \vec{x}^{new} = \vec{x}^{old} + \underset{1.2}{\wedge}\,\vec{v}^{old}\cdot\Delta t. \end{cases}$$

Han's version: 0.5, 1.2, ...

Need "Diagnostics" and output to do post-processing.

Results from simulation vs. Ground truth observation.

"We are solving the right eqn." ← (Validation)

vs. Theory / Analytical

"We are solving the eqn right" ← (Verification)

vs. Results from other simulations.

"Compare with others' results" ← (Benchmark)

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$$\left.\begin{array}{r} 3 = 5 \\ +\ 9 = 7 \end{array}\right\} \text{Algorithm.}$$

$$\overline{12 = 12} \quad \text{Results}$$

Back at 3:30 PM Central
1:30 PM Pacific.