Major Plasma Simulation Approaches and Publicly Available Simulation Codes

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Basic Numerical Descriptions

- Fluid Descriptions:
  - -Magnetohydrodynamics (MHD)
  - -Extended MHD: Including gravity, radiation, etc.
  - -Two-Fluid Description: Ions and electrons treated separately

- Kinetic Descriptions:
  - -Represent velocity space of each species: Six dimensional (3D-3V) phase space
  - -Velocity space can be represented by particles or on a fixed grid
  - -In magnetized plasmas, gyromotion can be averaged out: Gyrokinetics (3D-2V)
  - -Hybrid approaches: One species kinetically (ions) and one as a fluid (electrons)

MHD Simulations

- Magnetohydrodynamics (MHD) Equations (in conservative form)

Mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho \mathbf{v}] = 0, \quad (1)$$

Momentum
$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[\rho \mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} + \mathrm{P}^*\right] = 0, \quad (2)$$

Energy
$$\frac{\partial E}{\partial t} + \nabla \cdot \left[(E + P^*)\mathbf{v} - \mathbf{B}(\mathbf{B} \cdot \mathbf{v})\right] = 0, \quad (3)$$

Magnetic Induction
$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0, \quad (4)$$

Pressure Tensor
$$P^* = P + B^2/2$$

Energy
$$E = \frac{P}{\gamma - 1} + \frac{1}{2}\rho v^2 + \frac{B^2}{2}$$

- Requires closure by an Equation of State
  - -Connect pressure tensor to lower-order moments
  - -Ex: Ideal Gas $P = (\gamma - 1)e$
- MHD Simulations typically focus on
  - -Treatment of pressure tensor (isotropic, anisotropic)
  - -High spatial resolution (often using adaptive mesh)

Publicly Available MHD Simulation Codes

- Athena ++ https://princetonuniversity.github.io/athena/
  - -Astrophysical MHD code
  - -Flexible Coordinate Systems, including Adaptive Mesh Refinement (AMR)
  - -Radiation
  - -General Relativity
  - -Riemann Shock solver

- ZEUS-3D http://ap.smu.ca/~dclarke/zeus3d/version3.6/
  https://www.astro.princeton.edu/~jstone/zeus.html
  - -Early publicly available Radiation MHD code for astrophysics
  - -Widely used in the 1990s, 2000s
  - -Excellent series of code description and validation papers in *Astrophysical Journal Supplement*

Publicly Available MHD Simulation Codes

- FLASH http://flash.uchicago.edu/site/
  - -Modular, extensable system of codes
  - -MHD and Radiation with Adaptive Mesh Refinement
  - -Widely used for fluid studies of laser plasmas

- Many, many other MHD simulation codes are out there!

Kinetic Simulations

- Maxwell-Boltzmann Equations

Boltzmann equation for each species

$$\frac{\partial f_s}{\partial t} + \mathbf{v}\cdot\nabla f_s + \frac{q_s}{m_s}\left[\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right]\cdot\frac{\partial f_s}{\partial \mathbf{v}} = \left(\frac{\partial f_s}{\partial t}\right)_{\mathrm{coll}}$$

Maxwell's equations

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla\cdot\mathbf{E} = 4\pi\rho$$

$$\nabla\times\mathbf{B} = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} \qquad \nabla\cdot\mathbf{B} = 0$$

Charge Density

$$\rho = \sum_s \int d\mathbf{v}\ q_s f_s$$

Current Density

$$\mathbf{j} = \sum_s \int d\mathbf{v}\ q_s \mathbf{v} f_s$$

3D-3V Distribution Functions

$$f_s(\mathbf{r},\mathbf{v},t)$$

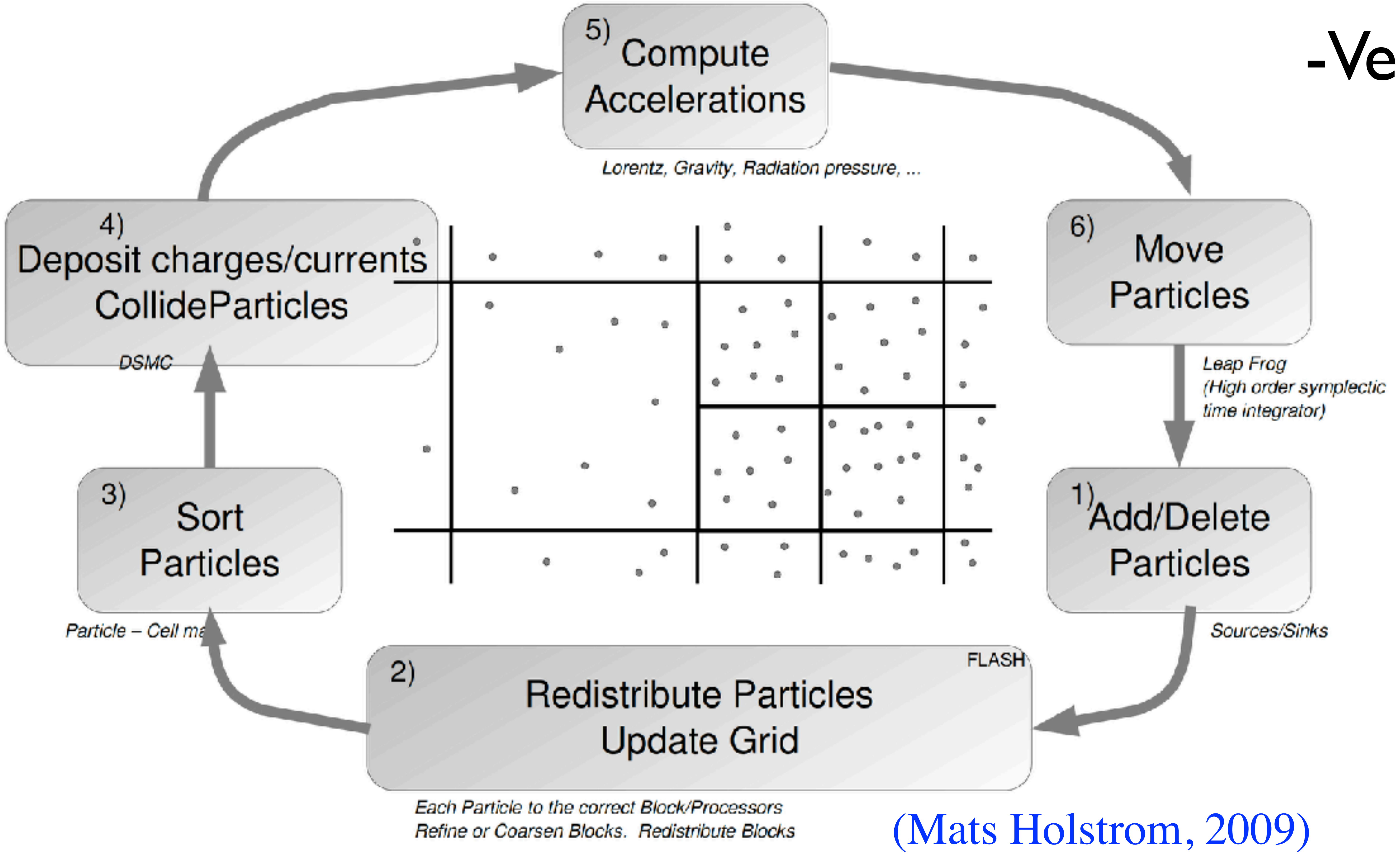
3D Electromagnetic Fields

$$\mathbf{E}(\mathbf{r},t) \qquad \mathbf{B}(\mathbf{r},t)$$

- Codes differ in how they choose to solve this system of equations numerically

Particle-in-Cell (PIC) Approach

- Basic Approach
  - -Charged particles are moved in fields (Lorentz Force Law)
  - -Electromagnetic fields are solved on a grid



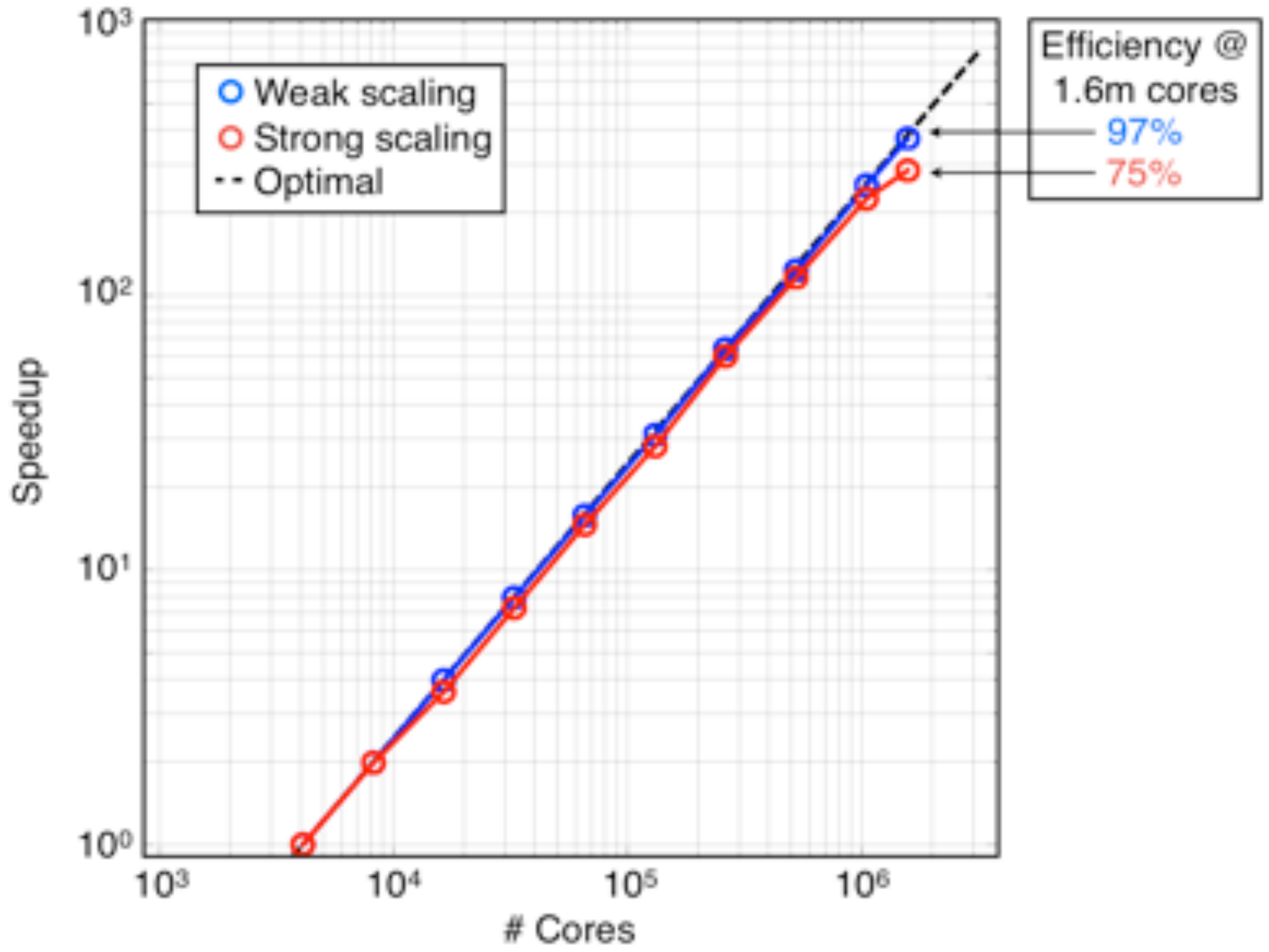
(Mats Holstrom, 2009)

-Very widely used in plasma physics

-Can be implemented very efficiently on supercomputers

Publicly Available PIC Simulation Codes

- OSIRIS   https://picksc.idre.ucla.edu
  - -Fully explicit, multidimensional, relativistic PIC code
  - -Supported by Particle-in-Cell and Kinetic Simulation Software Center at UCLA
  - -Highly optimized



Publicly Available PIC Simulation Codes

- VPIC https://github.com/lanl/vpic
  - -General purpose PIC code from Los Alamos National Laboratory
  - -Explicit, 2nd order leapfrog particle advance
  - -Highly optimized for parallel architectures

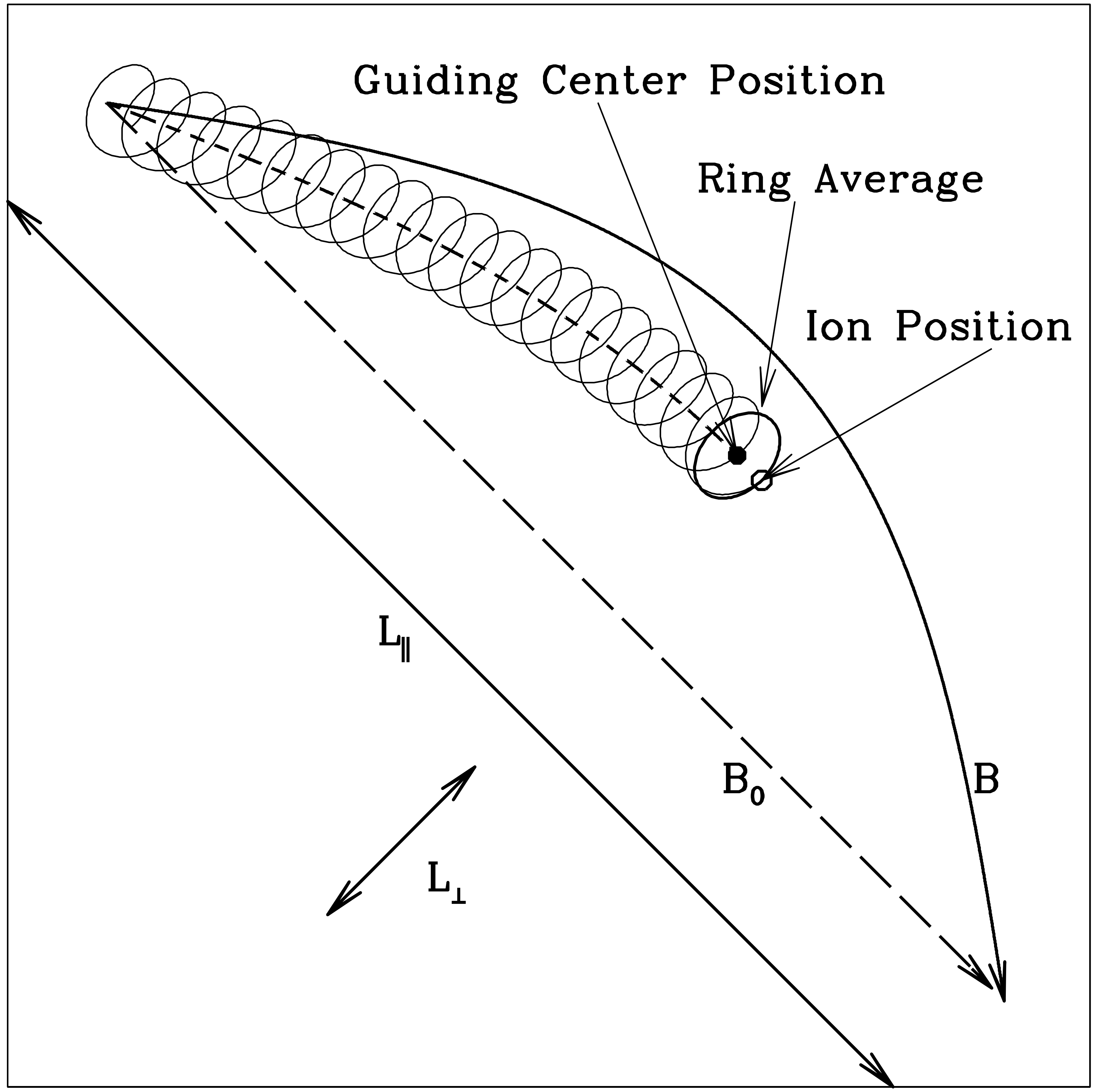
- iPIC3D http://www.allscale.eu/ipic3d
  https://github.com/CmPA/iPic3D
  - -Implicit PIC code for space weather applications
  - -Open source, C++ and MPI code

Gyrokinetic Approach

The University of Iowa

Gyrokinetics is kinetic theory averaged over the Larmor motion.

(Rutherford & Frieman 1968; Taylor & Hastie 1968; Frieman & Chen 1982; Howes et al. 2006)



(Howes *et al.*, ApJ **651**:590, 2006)

- Low-frequency limit eliminates fast cyclotron timescale $\omega \ll \Omega_i$
- Anisotropic $k_\parallel \ll k_\perp$
- Captures: Finite Larmor radius, Landau resonance, and Collisions
- Excludes: Fast wave and cyclotron resonance

Publicly Available Gyrokinetic Codes

- GS2/AstroGK/Trinity https://bitbucket.org/gyrokinetics/

  https://sourceforge.net/projects/gyrokinetics/

  -Family of gyrokinetic codes for fusion and astrophysical research
  -GS2 is a local gyrokinetic code for magnetic fusion research
  -Trinity is a global extension of GS2 for fusion research
  -AstroGK is a branch for the study of space and astrophysical plasmas

- GENE http://genecode.org

  -Open source plasma microturbulence code

- GTC http://phoenix.ps.uci.edu/GTC/

  -GyroPIC code (velocity space represented using particles)
  -Possibly outdated now

Hybrid Approach

- Basic Approach
  - -Treat ions as kinetic species (particles or on a grid)
  - -Treat electrons as a fluid
  - -Enables short electron timescales to be avoided, focusing on the timescales of the kinetic ion dynamics

Publicly Available Hybrid Codes

- HYB http://hyb.fmi.fi/index.php
  - -Developed at the Finnish Meteorological Institute
  - -Plasma interactions of planets, moons, comets and other celestial bodies

- HVM http://fis.unical.it/hvm/
  - -Hybrid Vlasov-Maxwell code
  - -Uses a velocity space grid for lower noise

- ANGIE 3D
  - -AuburN Global hybrId codE code
  - -For global simulations of the Earth's magnetosphere

Molecular Dynamics Approach

- Basic Approach
  - -N-Body approach where interactions between individual particles are explicitly modeled
  - -Can be used to explore strong coupling regime of plasmas
  - -Also can be used to explore 3D structure of proteins and other molecules

- LAMMPS https://lammps.sandia.gov
  - -Large-scale Atomic/Molecular Massively Parallel Simulator
  - -Used to model solid state (metals, semi-conductors)
  - -Used to model soft matter (biomolecules, polymers)

The End