Computational Methods for Fusion Science

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Agenda

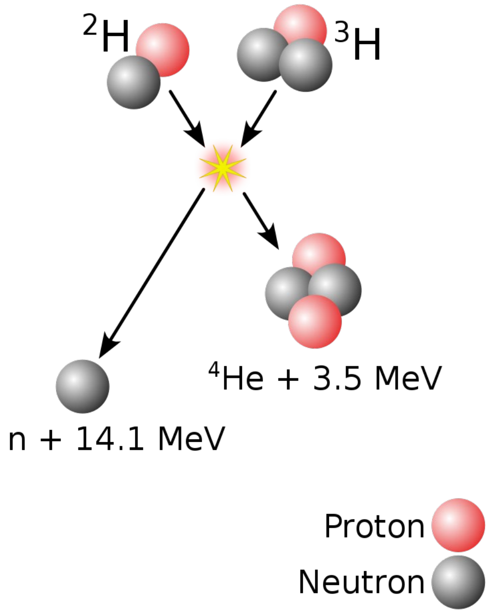
1. The quest for harnessing thermonuclear fusion as an energy source on Earth
2. Computing thermonuclear fusion: a very challenging endeavor
3. Computational methods for Magnetic Confinement Fusion
4. Computational methods for Inertial Confinement Fusion
5. A few examples of future research directions in Fusion Computation
6. Summary

Disclaimer: while I will attempt to provide as broad and as general a perspective on computing in Fusion Science as possible, my exposition will draw heavily from my own research and will reflect my personal perspective. Caveat emptor!

The quest for harnessing thermonuclear fusion as an energy source on Earth

What is thermonuclear fusion?

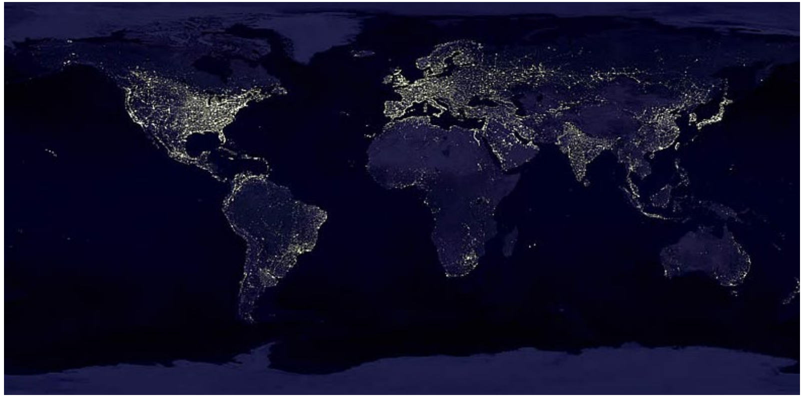
- " Thermonuclear Fusion" is the process whereby, upon reaching sufficiently high temperatures and densities, lighter nuclei combine to form heavier ones, converting a tiny amount of mass into a lot of energy (according to Einstein's mc^2 formula)
- Fusion is the engine that drives the birth, life, and death of stars in the universe, and therefore of life on Earth
  - In stars, matter is perfectly confined by gravity, allowing for long-term fusion energy production
  - In the laboratory, however, one needs to figure out ways to confine matter at billions of degrees hot… this is the key challenge of harnessing fusion on Earth!



Source: wikipedia

Why is thermonuclear fusion for peaceful energy production attractive?

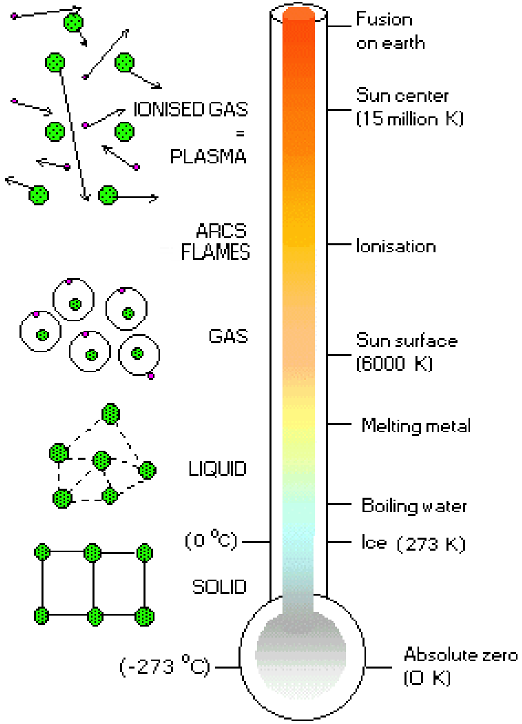
- Fuel is hydrogen isotopes: inexhaustible, geographically distributed
- Small quantity of fuel: quick shutdown
- Inherent safety aspects
- No harmful radioactive or CO_2 emissions (no global warming)
- Byproduct neutrons may activate structural materials, but next-generation fusion reactors will be “neutron-free”

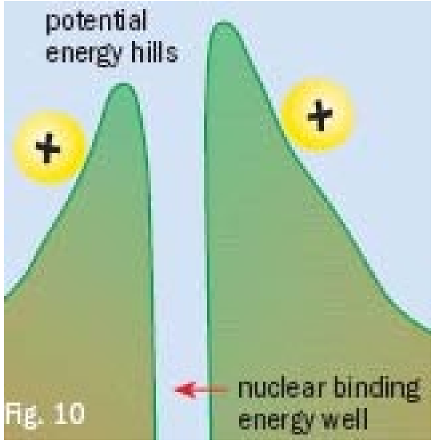


Only 100 kg deuterium (corresponding to 2800 tonnes of sea water) and 150 kg of tritium (corresponding to 10 tonnes of lithium ore) will be needed for operating a 1 GW electric power plant for one year.

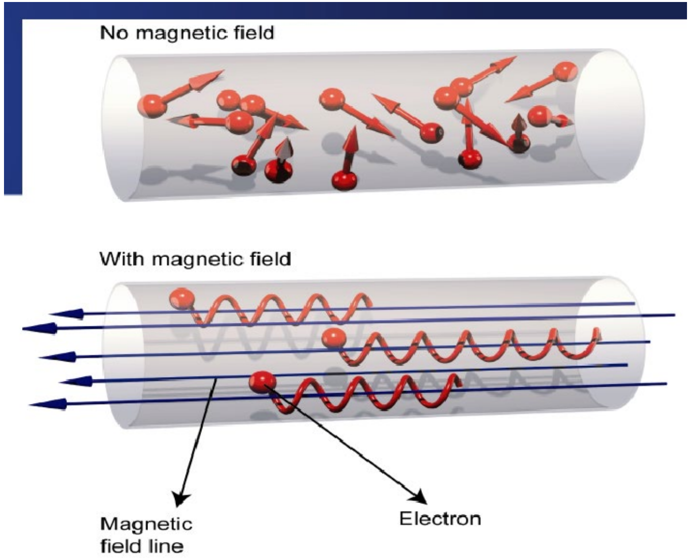
What are the required conditions for thermonuclear fusion?

- One hundred million degrees!
  - Enough kinetic energy to overcome electrostatic repulsion
- At such temperatures, matter is ionized and forms a **plasma** (4^{th} state of matter, most common!)
- Plasma is so hot it will instantly melt any surface: cannot come into contact with any reactor vessel! **Confinement.**

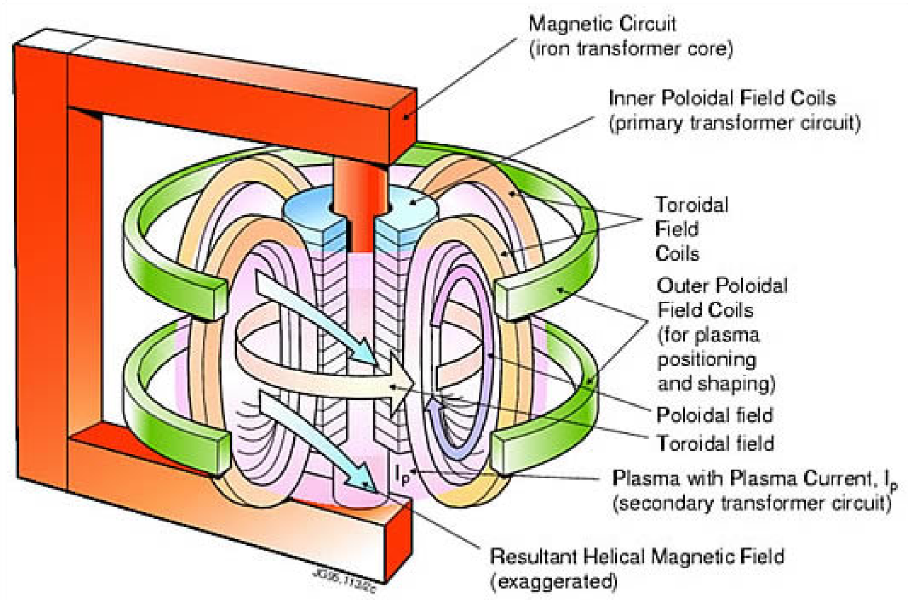




How to confine matter that hot?
I. With magnetic fields: Magnetic confinement

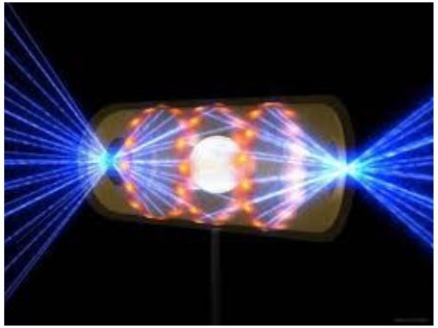


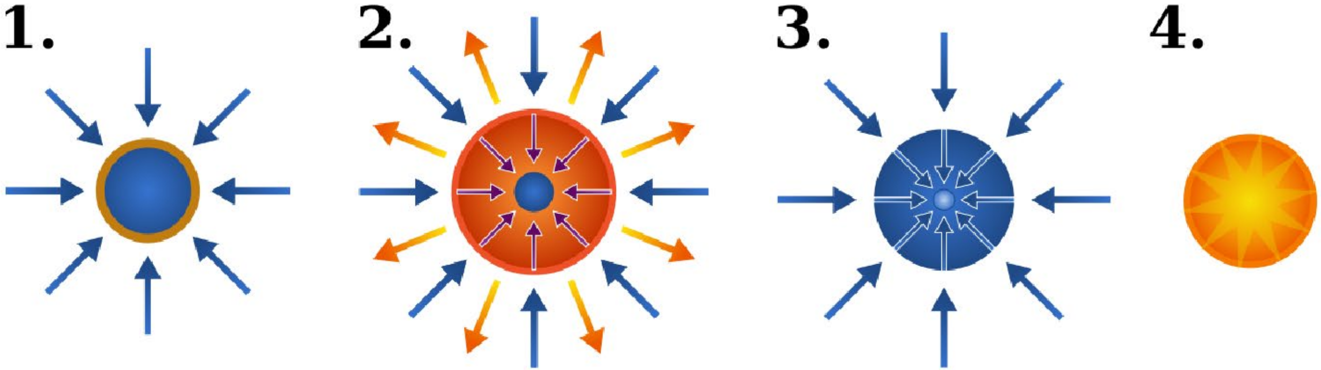
From W. Fox, PPPL



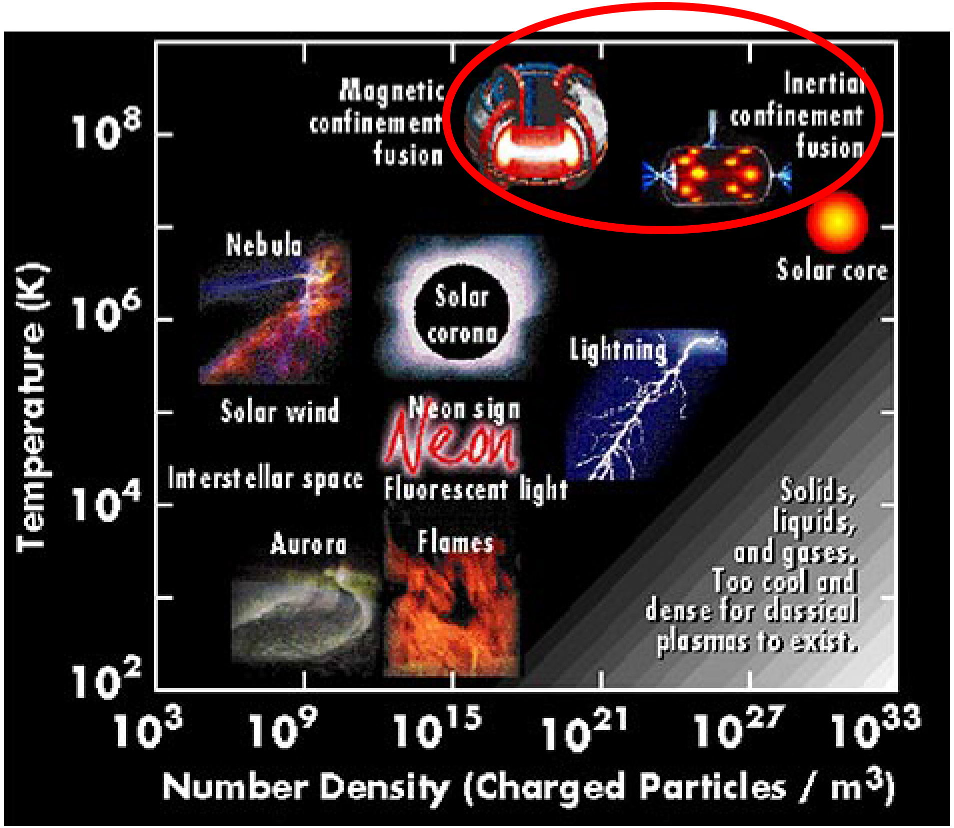
The toroidal geometry avoids end losses!

How to confine matter that hot?
II. By compression: Inertial confinement





A taxonomy of plasmas in nature and the laboratory



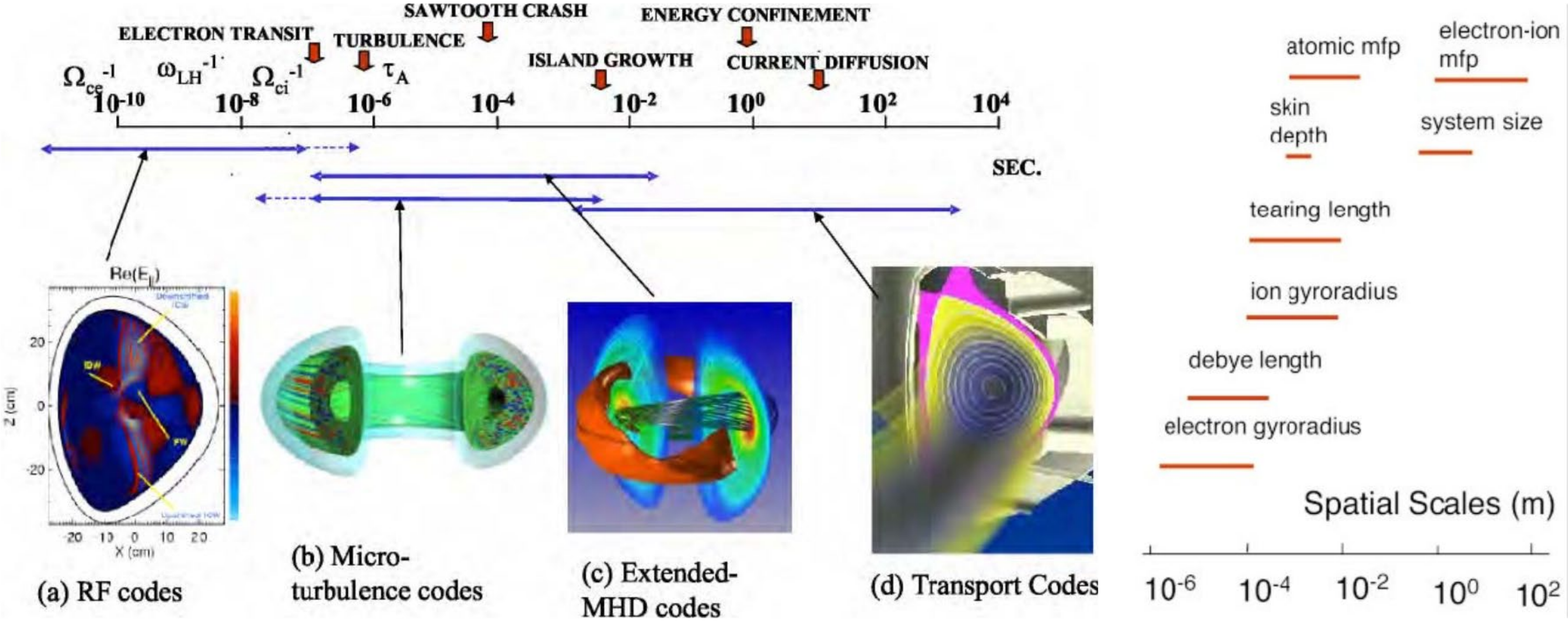
Simulating thermonuclear fusion: a very challenging endeavor

The role of computing in thermonuclear fusion: Virtual experiments

- Fusion experiments are getting bigger and more expensive: does not give room for iteration
- A successful fusion reactor should confine extremely hot matter at a sufficient density for sufficiently long: there is not much room for error!
- "Virtual experiments" are needed to find suitable operating regimes, and to guide construction, operation and optimization of future fusion reactors.
- Such "virtual experiments" are, or course, simulations. We require a predictive capability! However...

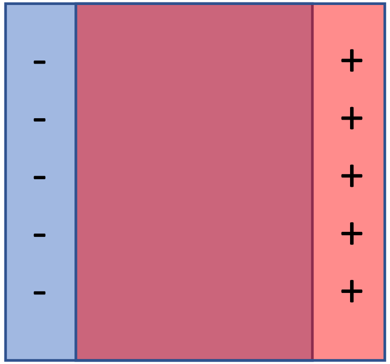
Plasma confinement (or lack thereof) results from careful interplay of physical phenomena spanning many orders of magnitude in time and space!

Challenges in thermonuclear fusion simulation: "The tyranny of scales"



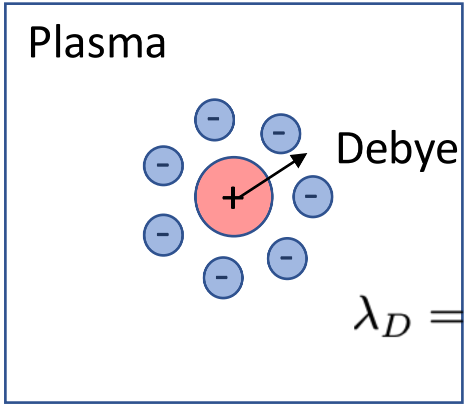
Challenges in thermonuclear fusion simulation: Charge separation characteristic scales

- Plasma frequency (very fast): time scale of restoration of charge imbalance in the plasma
- Debye length (very small): length scale beyond which charge separation cannot be sustained



$$\omega_p = \sqrt{\frac{q^2 n}{\epsilon_0 m}}$$

System tends to restore neutrality but overshoots, oscillating at plasma frequency

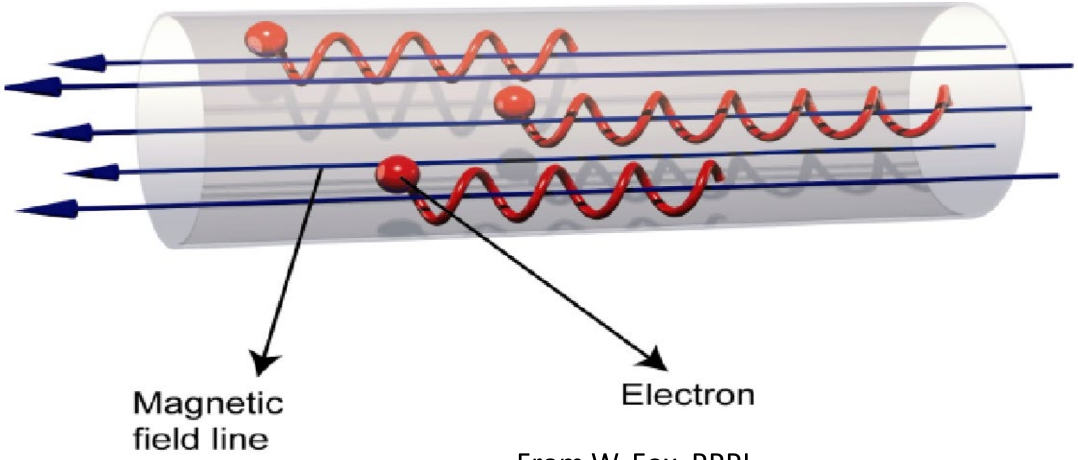


$$\lambda_D = \frac{v_{th}}{\omega_p} = \sqrt{\frac{\epsilon_0 T}{q^2 n}}$$

Electrons “shield” ion charge with characteristic scale the Debye length

Challenges in thermonuclear fusion simulation: Magnetic field characteristic scales

- Gyrofrequency (very fast): time scale of particle gyration around magnetic field
- Gyroradius (very small): radius of gyration around magnetic field



From W. Fox, PPPL

$$\Omega_c = \frac{qB}{m}$$

$$\rho_c = \frac{v_{th}}{\Omega_c} = \frac{\sqrt{mT}}{qB}$$

Challenges in thermonuclear fusion simulation: Collision frequencies and mean-free-paths

- Collision frequency:

$$\nu_c \propto \frac{q^4 n}{m^{1/2} T^{3/2}}$$

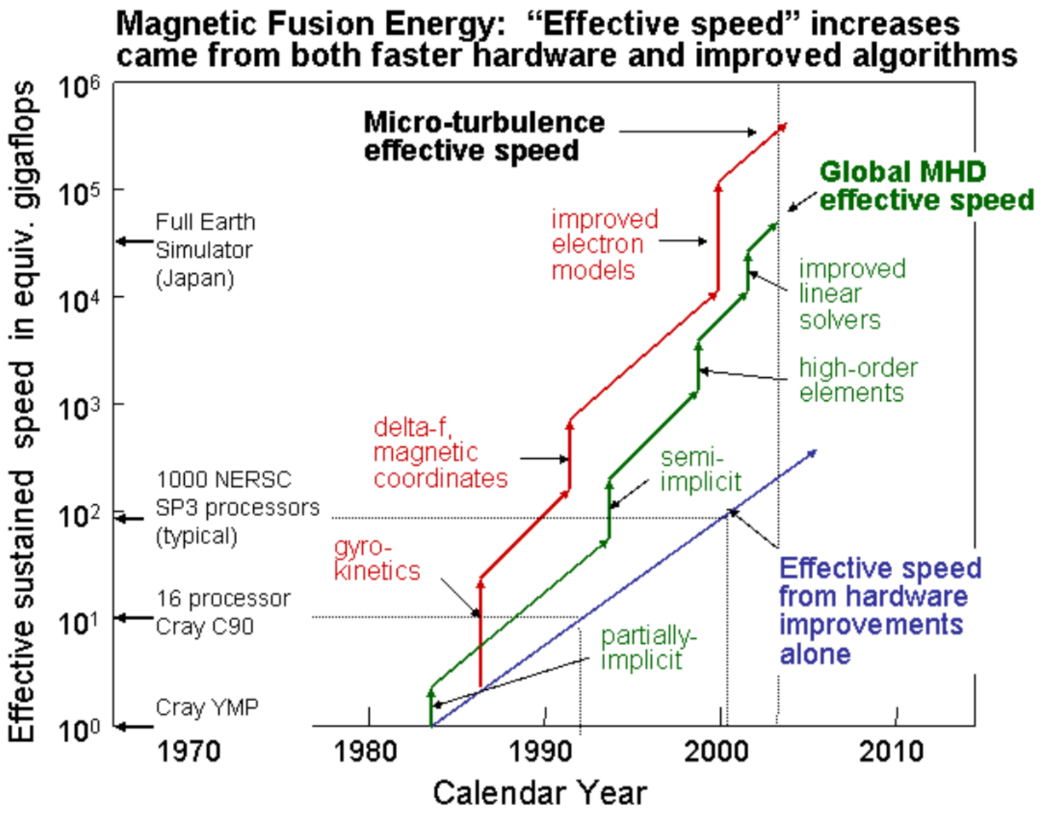
- Collisional mean-free-path: $\lambda_c = v_{th}/\nu_c$
- Collisions increase with density, decrease with temperature.
  - Hot, low-density plasmas are weakly collisional (MFE)
  - Warm, dense plasmas will be moderately or strongly collisional (ICF)
- Electrons are more collisional than ions by $\sqrt{m_i/m_e}$
- Collisions determine relaxation rates toward local thermal equilibrium (LTE)
- Collisionality affects momentum and energy transport, and therefore confinement.

Fusion sciences pioneered unclassified supercomputing!

- In 1973, Dr. Alvin Trivelpiece, deputy director of the Controlled Thermonuclear Research (CTR) program of the Atomic Energy Commission, solicited proposals for a computing center that would aid in reaching fusion power, giving the magnetic fusion program under CTR access to computing power similar to that of the defense programs.
- CTR computing center (CTRCC) was first placed at LLNL, and in 1996 moved to LBL.
- CTRCC was soon renamed "National Magnetic Fusion Energy Computing Center," and in 1983 adopted its final name of National Energy Research Supercomputing Center (NERSC) when it was open to al DOE-SC disciplines.

https://www.nersc.gov/about/nersc-history/?start=1

The power of algorithms!



Credit: S. Jardin, SCaLeS Report (2003)

The first-principles plasma description: Liouville's equation (an intractable problem)

- Evolution of particle distribution function (PDF) of N interacting particles with position $\mathbf{q}_i$ and momenta $\mathbf{p}_i$:

$$f_N = f_N(\mathbf{q}_1 \dots \mathbf{q}_N, \mathbf{p}_1 \dots \mathbf{p}_N, t)$$

- Is governed by the (6N+1) dimensionality equation:

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m} \frac{\partial f_N}{\partial \mathbf{q}_i} + \sum_{i=1}^{N} \mathbf{F}_i \frac{\partial f_N}{\partial \mathbf{p}_i} = 0,$$

- Note: N is the **real** number of physical particles!

Model reduction to the tractable: BBGKY hierarchy and the Boltzmann equation

- Define s marginal PDF by integrating over (s+1,…N) phase space:

$$f_s(\mathbf{q}_1 \dots \mathbf{q}_s, \mathbf{p}_1 \dots \mathbf{p}_s, t) = \int f_N(\mathbf{q}_1 \dots \mathbf{q}_N, \mathbf{p}_1 \dots \mathbf{p}_N, t)\, d\mathbf{q}_{s+1} \dots d\mathbf{q}_N\, d\mathbf{p}_{s+1} \dots d\mathbf{p}_N$$

- Leads to reduced equation:

$$\frac{\partial \boxed{f_s}}{\partial t} + \sum_{i=1}^{s} \frac{\mathbf{p}_i}{m} \frac{\partial \boxed{f_s}}{\partial \mathbf{q}_i} - \sum_{i=1}^{s} \left(\sum_{j=1 \neq i}^{s} \frac{\partial \Phi_{ij}}{\partial \mathbf{q}_i} + \frac{\partial \Phi_i^{ext}}{\partial \mathbf{q}_i} \right) \frac{\partial \boxed{f_s}}{\partial \mathbf{p}_i} = (N-s) \sum_{i=1}^{s} \int \frac{\partial \Phi_{i\, s+1}}{\partial \mathbf{q}_i} \frac{\partial \boxed{f_{s+1}}}{\partial \mathbf{p}_i} d\mathbf{q}_{s+1}\, d\mathbf{p}_{s+1}.$$

- "Closure problem": f_s depends on f_{s+1}
- Solution: close equation at s=1, and model rhs with collisions: **Boltzmann eq.**

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \frac{\partial f}{\partial \mathbf{q}} + \frac{\mathbf{F}}{m} \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t} \right)_c$$

- Still high dimensional (6D+time)!
- For grazing Coulomb collisions, Boltzmann reduces to the **Vlasov-Fokker-Planck-Landau equation**: basis for all fusion modeling!

A "tractable" first-principles model:
The Vlasov-Fokker-Planck equation (+ Maxwell Eqs)

$$\partial_t f_\alpha + \nabla_x \cdot (\vec{v} f_\alpha) + \nabla_v \cdot (\vec{a}_\alpha f_\alpha) = \sum_{\beta}^{N_s} \boxed{C_{\alpha\beta}\left(f_\beta, f_\alpha\right)} \qquad f = f\left(\vec{x}, \vec{v}, t\right)$$

$$\boxed{C\left(f_\beta, f_\alpha\right)} = \nabla_v \cdot \left[\boxed{\overline{\overline{D}}_\beta} \cdot \nabla_v f_\alpha - \boxed{\vec{A}_\beta} f_\alpha\right]$$

$$\boxed{\overline{\overline{D}}_\beta} = \nabla_v \nabla_v \boxed{G_\beta} \qquad \boxed{A_\beta} = \nabla_v \boxed{H_\beta}$$

$$\nabla_v^2 \boxed{H_\beta}\left(\vec{v}\right) = -8\pi f_\beta\left(\vec{v}\right)$$

$$\nabla_v^2 \boxed{G_\beta}\left(\vec{v}\right) = H_\beta\left(\vec{v}\right)$$

High dimensionality (3D+3V),
exceedingly multiscale

$+$

$$\partial_t \mathbf{B} + r \;\square\; \mathbf{E} = 0$$

$$-\mu_0 e_0 \partial_t \mathbf{E} + r \;\square\; \mathbf{B} = \mu_0 \mathbf{j}$$

$$r \cdot \mathbf{B} = 0$$

$$r \cdot \mathbf{E} = \frac{r}{e_0}$$

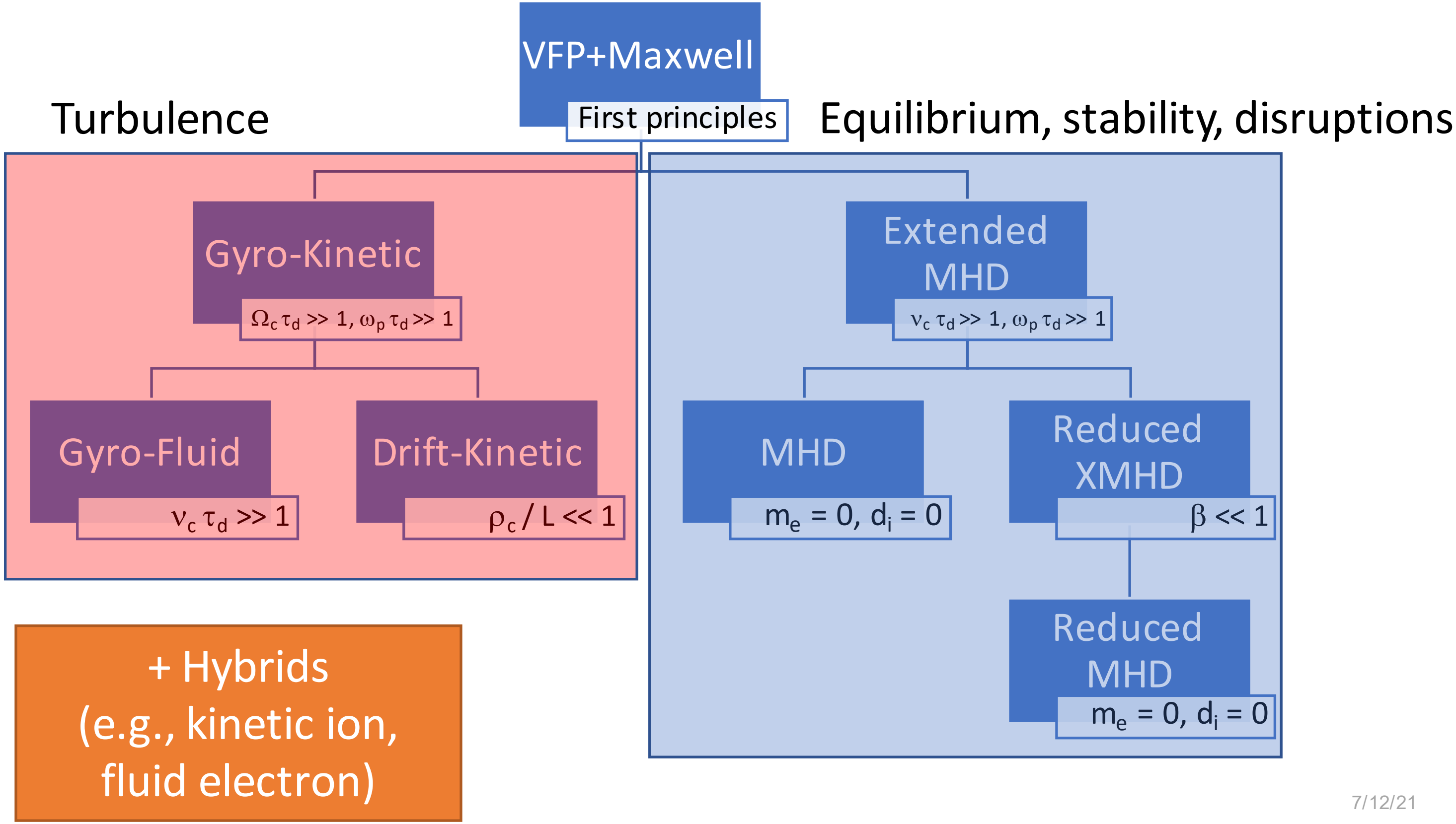
$$\rho(\mathbf{x}, t) = \sum_\beta q_\beta \int d\mathbf{v} f_\beta(\mathbf{x}, \mathbf{v}, t)$$

$$\mathbf{j}(\mathbf{x}, t) = \sum_\beta q_\beta \int d\mathbf{v} \;\; \mathbf{v} f_\beta(\mathbf{x}, \mathbf{v}, t)$$

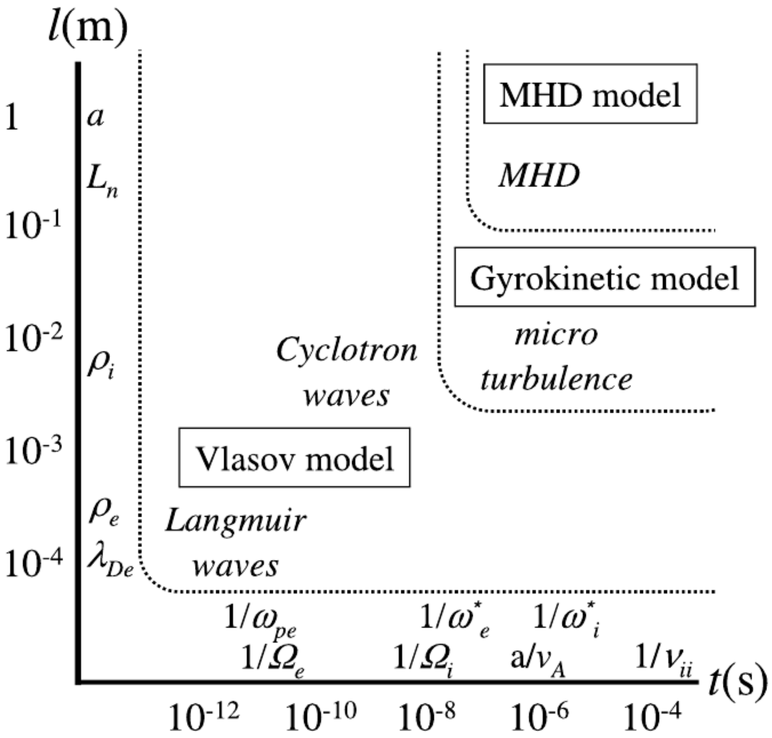
The power of asymptotics: nested model hierarchies

- Asymptotic model reduction from the VFP equation is possible by taking advantage of time/length scale separation
- In MFE, key asymptotic parameters are:
  - Plasma frequency ω_p (quasineutrality, ambipolarity)
  - Gyrofrequency Ω_c, the gyroradius ρ_c (magnetic field strength)
  - Collision frequency ν_c and mean-free-path λ_c (plasma collisionality)
  - Ion/electron skin depths, $d_{i,e}=c/\omega_{p\,i,e}$ (measure scale lengths where kinetic effects are important)
- In ICF, key asymptotic parameters are:
  - Plasma frequency
  - Plasma collisionality and mean-free-path
  - Plasma β (ratio of thermal-to-magnetic pressures)

Model hierarchy in MFE

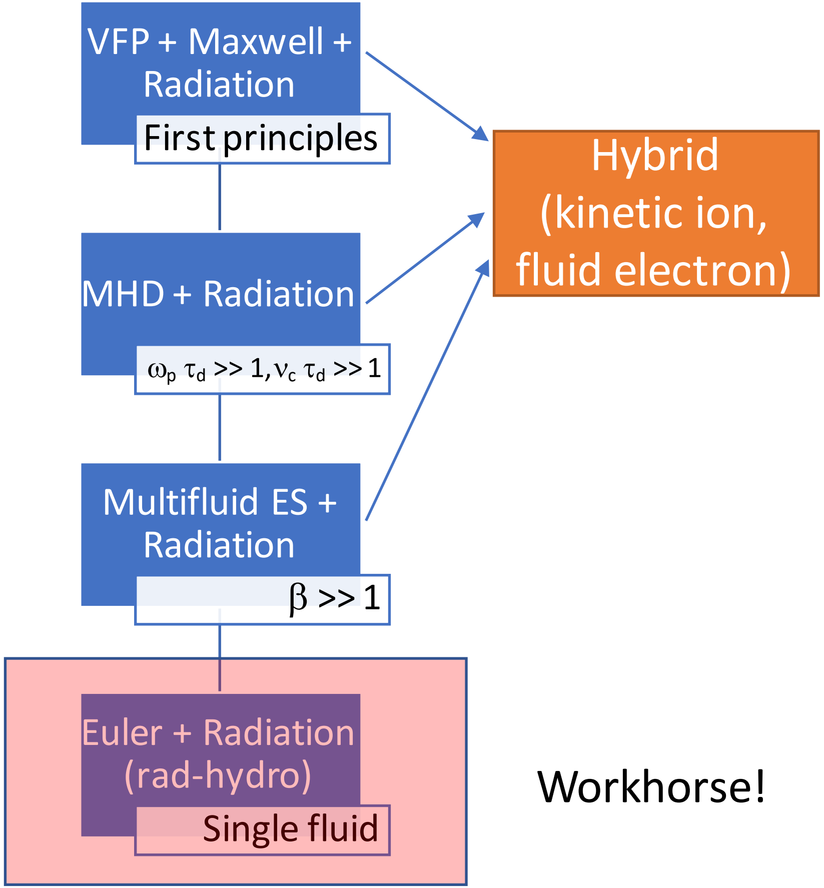


Model hierarchy in MFE



Credit: Grandgirard

Model hierarchy in ICF

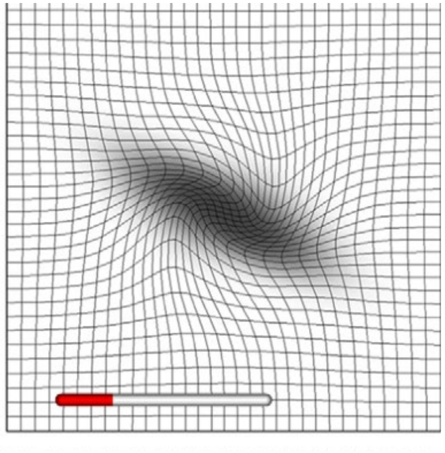


Workhorse!

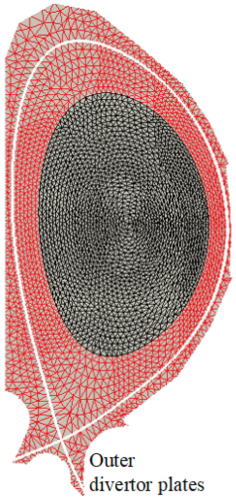
A taxonomy of computational methods for fusion science

- **Spatial discretization**
  - Lagrangian
  - Eulerian
  - Spectral (e.g., Fourier in periodic directions)
  - Hybrid (e.g., particle-in-cell)
- **Temporal discretization**
  - Implicit
  - Explicit
  - Hybrid (e.g., IMEX)
- **Model fidelity**
  - Fluid
  - Kinetic
  - Hybrid (e.g., Kinetic-ion/fluid-e)

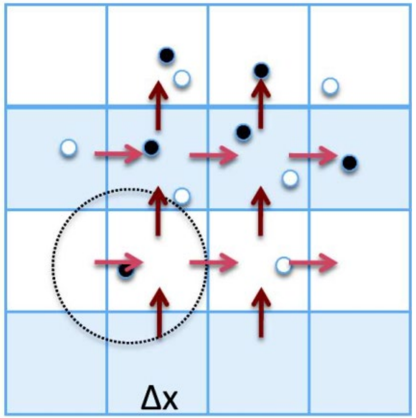
Spatial discretization approaches



Lagrangian



Eulerian



Hybrid

Temporal discretization approaches

$$\frac{\partial \Phi}{\partial t} = D\Delta\Phi$$

- Explicit
- Implicit-Explicit (IMEX)
- Implicit

$$\Phi^{n+1} = \Phi^{n} + \Delta t D \Delta \Phi^{n}$$

Easy update (no solve), conditional stability on Δt

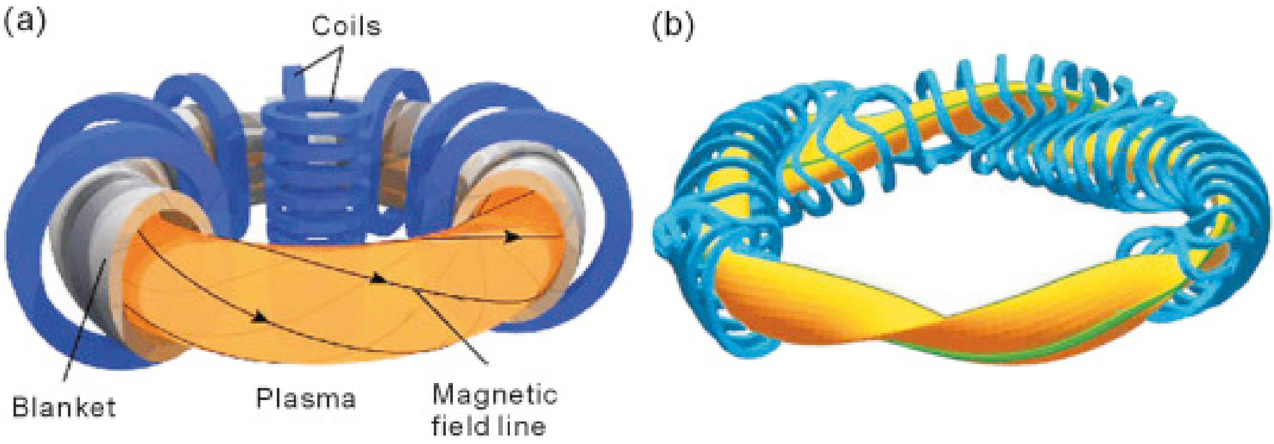
$$\Phi^{n+1} = \Phi^{n} + \Delta t D \Delta \Phi^{n+1}$$

Requires global algebraic solve (hard), unconditionally stable in Δt

Computational methods for Magnetic Confinement Fusion

What is magnetic confinement fusion?

- Magnetic confinement fusion (also known as Magnetic Fusion Energy, MFE) attempts to “bottle” million-degree hot plasma using magnetic fields.
- Leading concepts are based on toroidal geometries (no end losses)
  - Best known concept is **tokamak**, in which the plasma generates confining poloidal magnetic fields self-consistently with plasma currents.
  - Other fusion-grade concepts include the **stellarator**, which creates confining magnetic fields with external coils.



Magnetohydrodynamics (MHD): equilibrium and stability

- MHD describes well macroscopic (bulk) plasma behavior.
- A self-sustaining long-pulse (quasi-steady-state) MFE reactor must be:
  - In MHD equilibrium: $\mathbf{j} \times \mathbf{B} \approx \mathrm{grad}(P)$
  - MHD stable (perturbations to the equilibrium must decay, not grow exponentially)
- MHD toroidal equilibrium can be 2D or 3D, and must satisfy $\mathbf{j} \times \mathbf{B} = \mathrm{grad}(P)$
  - 2D equilibria are computed using the Grad-Shafranov equation [reduction of $\mathbf{j} \times \mathbf{B} = g(P)$]
  - 3D equilibria requires solving full MHD equilibrium equation (e.g., in stellarator)
- MHD stability is critical for long-term reactor operation
  - Stellarator concept does not self-generate magnetic fields, and is MHD-robust
  - Tokamak stability is more nuanced. If plasma becomes unstable in a tokamak, the plasma may terminate, causing a DISRUPTION. This should be avoided at all costs.

The MHD model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0,$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[\rho \mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} + \overleftrightarrow{\Pi} + \overleftrightarrow{I}\left(p + \frac{B^2}{2}\right) \right] = 0,$$

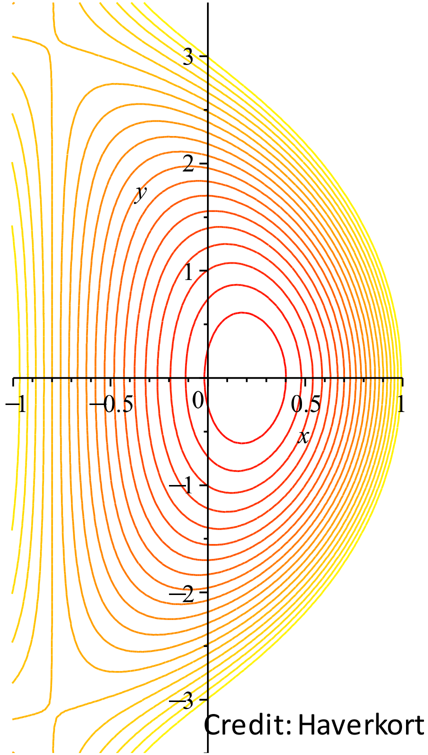
$$\frac{\partial p_e}{\partial t} + \nabla \cdot (\mathbf{v} p_e) + (\gamma - 1) p_e \nabla \cdot \mathbf{v} = (\gamma - 1)(S - \nabla \cdot \mathbf{q}).$$

$$\mathbf{v} = \frac{m_i \mathbf{v}_i + m_e \mathbf{v}_e}{m_i + m_e} \approx \mathbf{v}_i \; ; \; \mathbf{v}_e = \mathbf{v}_i - d_i \frac{\mathbf{J}}{\rho}$$

$$\text{Ohm's Law}: \mathbf{E} = -\mathbf{v} \times \mathbf{B} + \eta \mathbf{J} - \frac{d_i}{\rho}\left(\mathbf{J} \times \mathbf{B} - \nabla p_e - \nabla \cdot \overleftrightarrow{\Pi}_e\right) - \frac{d_e^2}{d_i} \frac{d\mathbf{v}_e}{dt}$$

MHD equilibrium: Grad-Shafranov equation

- Goal is to find poloidal flux $\Psi(x)$ for a given toroidal magnetic field $F=R\,B_\phi=F(\Psi)$ and pressure profile $p(\Psi)$ such that: $$\nabla \cdot \left(\frac{\nabla\Psi}{R^2}\right) = -\frac{dp}{d\Psi} - \frac{F}{R^2}\frac{dF}{d\Psi}$$
- Magnetic field is found from: $\mathbf{B} = \nabla\Psi \times \nabla\phi + F\nabla\phi$
- Highly nonlinear equation! Can be very difficult to solve.
  - Discretized using FV, FD, FE, spectral methods.
  - Requires nonlinear iteration
  - Input functions $p(\Psi)$, $F(\Psi)$ can be eliminated by adding more physics (for instance, loop voltage and resistive decay), or can be provided in alternative forms
  - Many available codes: EFIT, TEQ, CORSICA, CHEASE
- Codes that solve 3D MHD equilibria (stellarator) also exist: PIES (3D), VMEC (3D)



Credit: Haverkort

MHD stability: Methods

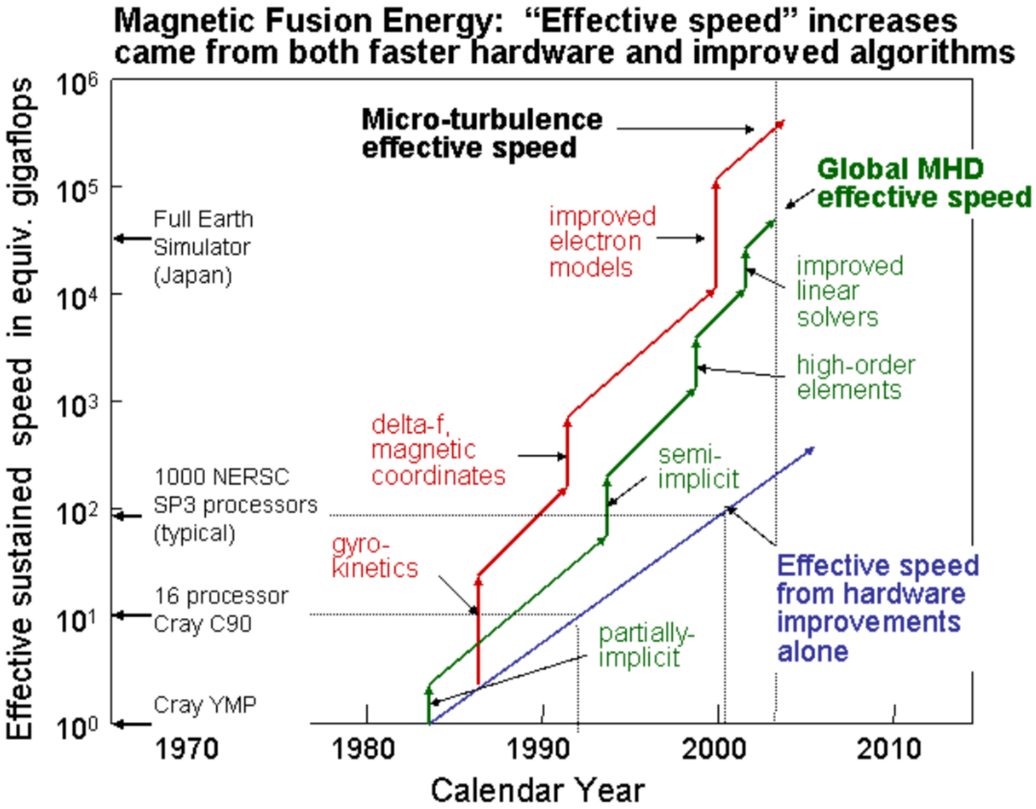
- After an equilibrium is found, it is important to determine whether it is MHD stable or unstable
- The question of stability is a tiered one: ideal stability (without dissipation), resistive stability, two-fluid stability, kinetic stability….
- There are many specialized tools to determine MHD stability, including some beyond-MHD effects:
  - DCON (extended Newcomb's criterion)
  - PEST (MHD energy principle)
  - MARS (spectral)
  - ELITE (edge localized modes)
  - …
- Initial-value MHD computations by full-fledged MHD codes are also used to study MHD stability

MHD initial-value simulations of MFE: Methods

- MHD is a hyperbolic PDE system, supporting a variety of fast waves (fast and slow magnetosonic, shear Alfven).
- Spatial discretizations: FV, FD, FE, spectral,…
- Temporal discretizations: semi-implicit, fully implicit
  - MFE benefits from quiescent plasmas, and therefore MHD simulations may need to cover a very long time span
  - Resolving fast timescales is impractical: implicit timestepping ($\Delta t\, \omega_{MHD} >> 1$)
  - Many MHD codes are available for MFE (NIMROD, M3D-C1, PIXIE3D, JOREK, SpeCyl, HiFi,…). All of them feature some level of time-implicitness.
  - Key algorithmic requirement: SCALABILITY
- Achieving algorithmic and parallel scalability in implicit MHD codes is difficult
  - Algorithmic scalability: CPU ~ O(N log(N)), N: number of degrees of freedom
  - Parallel scalability: CPU ~ $1/N_p$, N_p: number of processors
  - We need **both**!

MHD: Impact of algorithms

- Impact both from spatial and temporal discretization improvements
  - High-order, mesh adaptivity, etc.
- Time-implicitness is key
- Suitable linear and nonlinear solvers to invert associated algebraic system of equations is also important for scalability
- MHD algorithms remain an active area of research



Credit: S. Jardin, SCaLeS Report (2003)

MHD: Implicit timestepping algorithms
Why are they so difficult to scale up?

- Implicit timestepping requires an algebraic (often nonlinear) solve:

$$G(U^{n+1}) = U^{n+1} - U^n - \Delta t F(U^{n+1}) = 0 \quad ; \quad U = [\rho, \mathbf{v}, p]$$

- G(U) is generally nonlinear, and requires iteration, e.g. Newton-Raphson

$$\left.\frac{\partial G}{\partial U}\right|_k \delta U_k = -G(U_k) \quad ; \quad U_{k+1} = U_k + \delta U_k$$

- Jacobian matrix $J_k = \partial G/\partial U_k$ is a very large, sparse, ill-conditioned matrix
  - Direct methods are prohibitive [e.g., Gaussian elimination, CPU~ O($N^{7/3}$) in 3D!]
  - Requires iterative methods, but typically # iterations grows with the condition number of the matrix: not scalable!
- Solution: Multigrid-preconditioned Krylov methods

Krylov methods: a primer

- Krylov methods attempt to find the solution of **Ax=b** as a series: $\mathbf{x} = \sum_i a_i \mathbf{d}_i$
- Here, $\mathbf{d}_i$ are A-conjugate vectors, satisfying orthogonality property:

$$\mathbf{d}_i A \mathbf{d}_j = \delta_{ij} \Rightarrow a_i = \mathbf{d}_i^T \mathbf{b}$$

- Problem solved! Right? No… one needs to find conjugate vectors!
- Krylov methods build conjugate basis iteratively, and orthogonalize along the way (e.g., Gram-Schmidt, QR factorization, etc.):

$$\{\mathbf{r}, A\mathbf{r}, A^2\mathbf{r}, \ldots\} \rightarrow \{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \ldots\}$$

  - All that is required to form basis is to multiply matrix A times a (given) vector once per iteration!
  - For Jacobian system (Newton), matrix-vector product can be performed without ever building and storing the Jacobian matrix! (Gateaux derivative)

$$\left.\frac{\partial \vec{G}}{\partial \vec{x}}\right|_k \vec{y} = J_k \vec{y} = \lim_{\epsilon \to 0} \frac{\vec{G}(\vec{x}_k + \epsilon \vec{y}) - \vec{G}(\vec{x}_k)}{\epsilon}$$

Preconditioning Krylov methods

- Krylov methods are much faster than other iterative methods (e.g., Jacobi, Gauss-Seidel), but still not optimal. But they can be PRECONDITIONED!
- Preconditioning: rewrite linear system as:

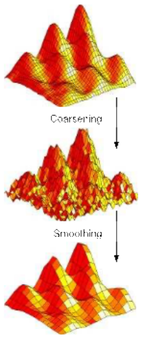
$$AP^{-1}Px = b \Rightarrow (AP^{-1})y = b \quad ; \quad x = P^{-1}y$$

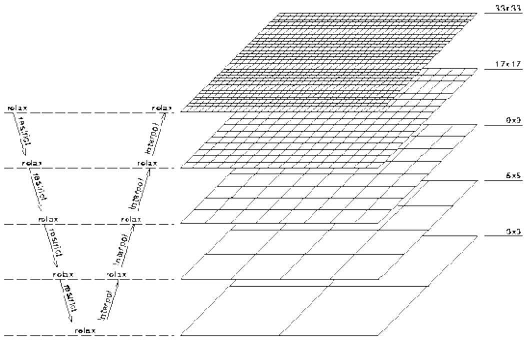
P^{-1} is the preconditioner. If $P^{-1} \sim A^{-1}$, then $(A P^{-1}) \sim I$, very fast convergence!

- Matrix-vector multiplication feature of Krylov methods allow seamless implementation of preconditioner:
  - $z=(A P^{-1})v$ can be computed with 2 matrix-vector products: $y= P^{-1}v$, $z = Ay$
- Bleeding-edge research in iterative methods is in the development of effective preconditioners
  - Preconditioner only affects convergence, not the solution
  - Approximations to PDE that would lead to bad solvers can be good preconditioners!
  - Application dependent

Multigrid methods

- MG employs a divide-and-conquer approach to attack error components in the solution
  - Oscillatory components of the error are “EASY” to deal with (if a SMOOTHER exists)
  - Smooth components are DIFFICULT
- MG idea: coarsen recursively to make “smooth” components become oscillatory





- SMOOTHER is KEY component of MG
- Smoother for stiff hyperbolic equations are hard to formulate
- However, smoother for parabolic systems are much easier to develop: PARABOLIZATION of stiff hyperbolic PDEs

Parabolization of stiff hyperbolic systems: Physics-based multigrid preconditioning

- Parabolization enables development of effective preconditioners for stiff hyperbolic PDEs
  - Parabolization exploits structure of implicit discretization

$$\partial_t u = \frac{1}{\epsilon}\partial_x v \,,\ \partial_t v = \frac{1}{\epsilon}\partial_x u.$$

$$u^{n+1} = u^n + \frac{\Delta t}{\epsilon}\partial_x v^{n+1}, v^{n+1} = v^n + \frac{\Delta t}{\epsilon}\partial_x u^{n+1}.$$

$$\Rightarrow \boxed{\left[I - \left(\frac{\Delta t}{\epsilon}\right)^2 \partial_{xx}\right] u^{n+1} = u^n + \frac{\Delta t}{\epsilon}\partial_x v^n}$$

  - Parabolized systems are suitable for modern multilevel solvers (multigrid), which can be optimal [CPU ~ O(N log(N))]

- Connection between parabolization and block-factorization (Schur complement):

$$\begin{bmatrix} D_1 & U \\ L & D_2 \end{bmatrix} = \begin{bmatrix} I & UD_2^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} D_1 - UD_2^{-1}L & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} I & 0 \\ D_2^{-1}L & I \end{bmatrix}$$

$$D_1 - UD_2^{-1}L = \left[I - \left(\frac{\Delta t}{\epsilon}\right)^2 \partial_{xx}\right]$$

- Provides path for application of parabolization strategy to complex stiff hyperbolic PDEs.

Jacobian-free Newton-Krylov + Parabolization delivers near-optimal scalability (parallel and algorithmic)

- Hall MHD example using GEM challenge problem (magnetic reconnection)
- Fixed implicit timestep, weak-scalability study

np	mesh	n_e	$\frac{Dt}{Dt_{exp}}$	GMRES/ Dt	Newton/ Dt	WCT(s)	WCT/ PC
1	32 □ 32	10^{-4}	1.0	2	2	174	43.5
4	64 □ 64	2.5 □ 10^{-5}	2.1	2	2	214	53.5
16	128 □ 128	6.3 □ 10^{-6}	8.2	2	2	298	74.5
64	256 □ 256	1.6 □ 10^{-6}	170	7	3.8	1030	95.4
256	512 □ 512	3.9 □ 10^{-7}	130	3.2	2.4	648	115.7
1024	1024 □ 1024	9.8 □ 10^{-8}	520	2.9	2.4	961	181.3
4096	2048 □ 2048	2.4 □ 10^{-8}	2100	4.1	2.7	1350	198.5

Application: [redacted] (PIXIE3D)

[redacted] Disruption Simulation
[redacted]roject (PI: X. Tang, LANL)

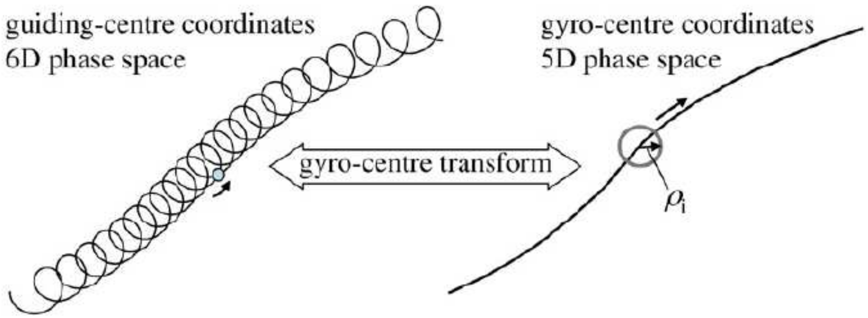
Beyond MHD: GK and micro-turbulence in tokamaks

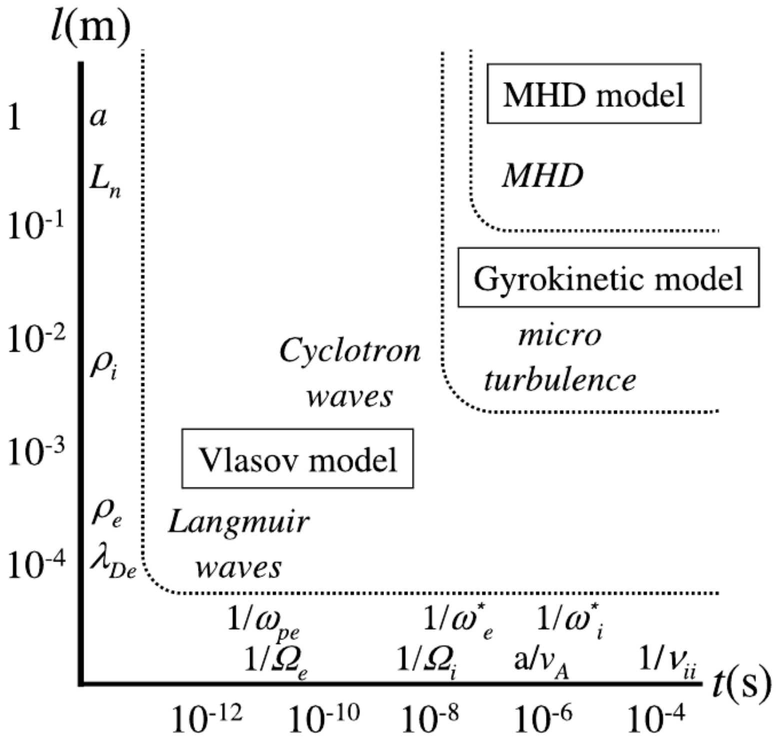
- For MHD-stable magnetic-field tokamak configurations, small-scale (kinetic) instabilities develop that lead to micro-turbulence (both electrostatic and electromagnetic)
- Micro-turbulence has huge impact on particle and energy confinement in tokamaks
- Requires a kinetic description: Gyrokinetics
  - Enforces quasineutrality
  - Exploits that gyrofrequency is very fast, and gyrophase angle ignorable
  - Does NOT assume gyroradius is too small (turbulence can in fact develop spatial scales comparable to ion and electron gyroradii)
- Gyrokinetics is one of the most successful asymptotic models in MFE
  - Spatial discretization: both particle-in-cell and Eulerian.
  - Temporal discretization: semi-implicit.
  - Fully implicit methods are being actively developed.

Gyrokinetic (GK) model reduction

- Fast gyro-motion is averaged out

$$f(\mathbf{x}, v_{\|}, v_{\perp}, \varphi_c, t) \rightarrow \bar{f}(\mathbf{x}_G, v_{G\|}, \mu, t)$$





GK: an algorithmic revolution

- Goal: analytically remove fast plasma and gyro-frequencies (asymptotic model)
- Results in dimensionality reduction (5D instead of 6D)
- ”delta-f” representations focus the numerical representation on deviations from Maxwellian (local thermal equilibrium)

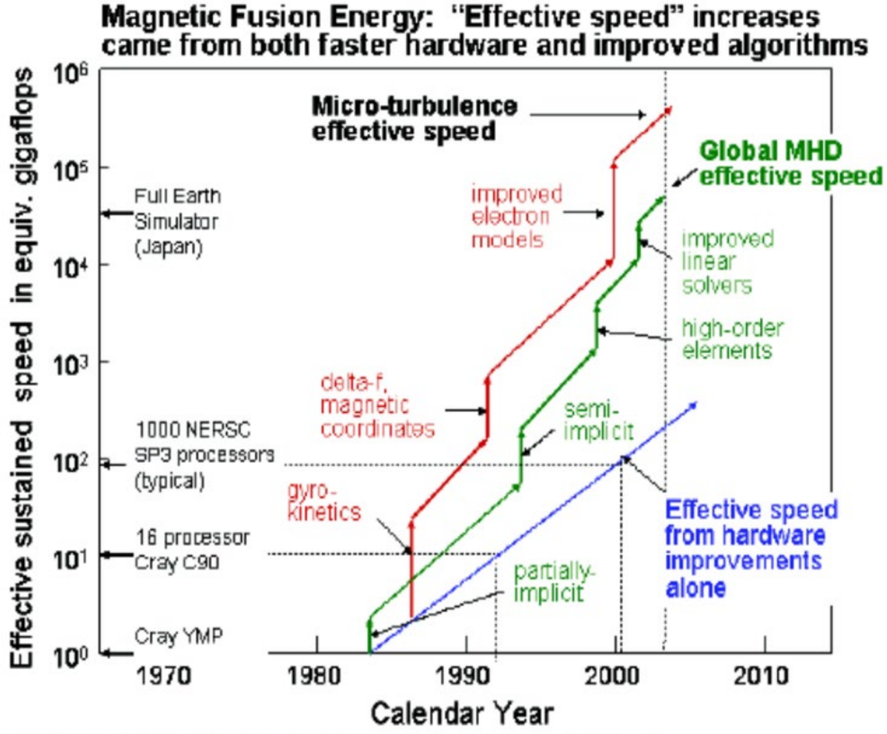


Figure from SCaLeS report, Volume 2 (2004), c/o S. Jardin

GK equations

- Transport equation

$$\frac{\partial f_s}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f_s}{\partial \mathbf{X}} + \dot{v}_\parallel \frac{\partial f_s}{\partial v_\parallel} = 0 \qquad f_s(\mathbf{X}, \mu, v_\parallel, t) : \mathbb{R}^5 \times \mathbb{R} \to \mathbb{R}^+$$

$$\dot{\mathbf{X}} = \frac{1}{D}\left[v_\parallel \left(\hat{\mathbf{b}}_0 + \delta \hat{\mathbf{b}} \right) + \frac{m_s}{q_s B_0} v_\parallel^2 \nabla \times \hat{\mathbf{b}}_0 - \frac{m_s}{q_s B_0} \hat{\mathbf{b}}_0 \times \left(\frac{q_s}{m_s} \langle \mathbf{E} \rangle - \mu \nabla B_0 \right) \right]$$

$$\dot{v}_\parallel = \frac{q_s}{m_s D} \left[\left(\hat{\mathbf{b}}_0 + \delta \hat{\mathbf{b}} \right) + \frac{m_s}{q_s B_0} v_\parallel \nabla \times \hat{\mathbf{b}}_0 \right] \cdot \left(\langle \mathbf{E} \rangle - \frac{m_s}{q_s} \mu \nabla B_0 \right)$$

$$D = 1 + \frac{m_s}{q_s B_0} v_\parallel \mathbf{b}_0 \cdot \nabla \times \mathbf{b}_0$$

- Field equations

$$-\frac{e n_0 m_i}{q_i B_0^2} \nabla_\perp^2 \phi = q_i \bar{n}_i - e n_e$$

$$-\frac{1}{\mu_0} \nabla_\perp^2 A_\parallel = j_{\parallel i} + j_{\parallel e}$$

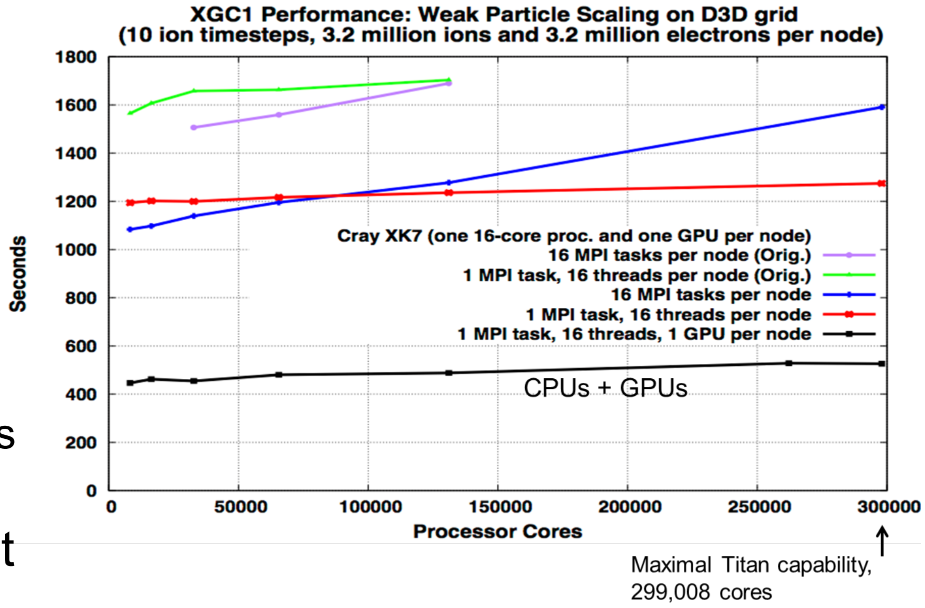
$$\bar{n}_i(\mathbf{x}) = \int_{-\infty}^{\infty} \int_0^{\infty} \left\langle f_i(\mathbf{X}, v_\parallel, \mu) \delta(\mathbf{X} - \mathbf{x} + \boldsymbol{\rho}_i) \right\rangle B d\mu dv_\parallel$$

$$n_e(\mathbf{x}) = \int_{-\infty}^{\infty} \int_0^{\infty} \left\langle f_e(\mathbf{X}, v_\parallel, \mu) \delta(\mathbf{X} - \mathbf{x}) \right\rangle B d\mu dv_\parallel$$

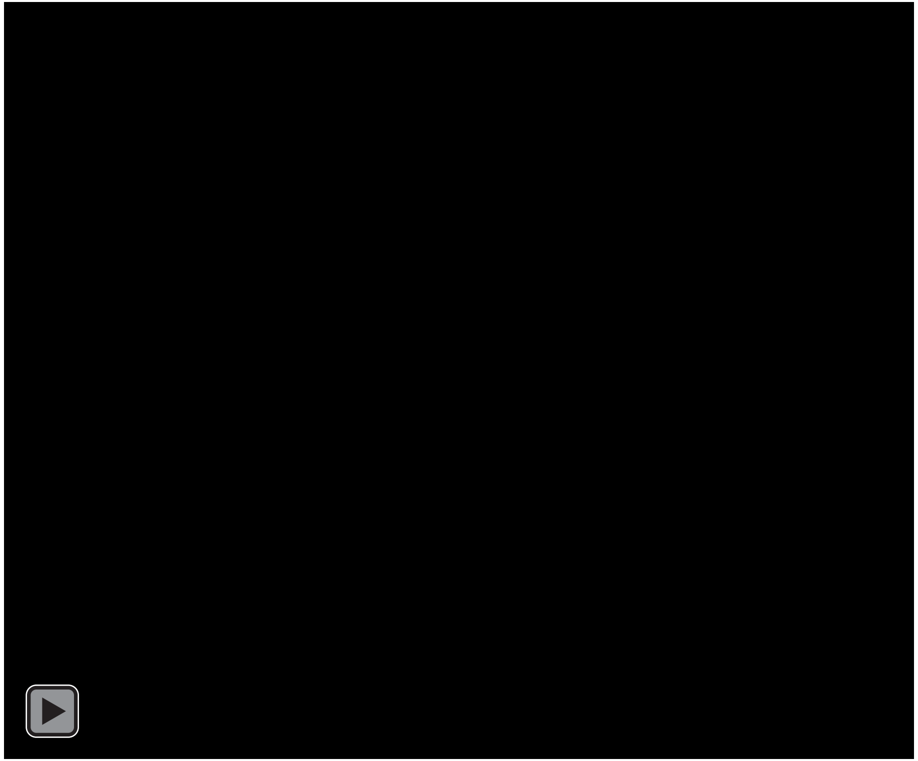
$$j_{\parallel s}(\mathbf{x}) = q_s \int_{-\infty}^{\infty} \int_0^{\infty} v_\parallel \left\langle f_s(\mathbf{X}, v_\parallel, \mu) \delta(\mathbf{X} - \mathbf{x}) \right\rangle B d\mu dv_\parallel$$

The gyro-kinetic model: methods

- Spatial discretizations (configuration space): FD, FE, spectral…
- Velocity space discretizations:
  - Mesh
  - Particles (PIC)
- Temporal discretization: semi-implicit
  - Accuracy issues (cancellation problem)
  - Ongoing research on fully implicit methods to resolve
- GK codes can effectively use the largest HPC computers on Earth!



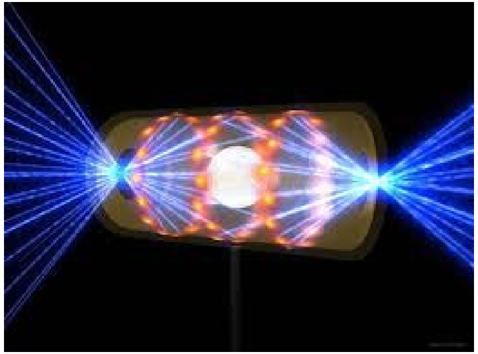
A GK turbulence simulation of the tokamak edge (XGC)

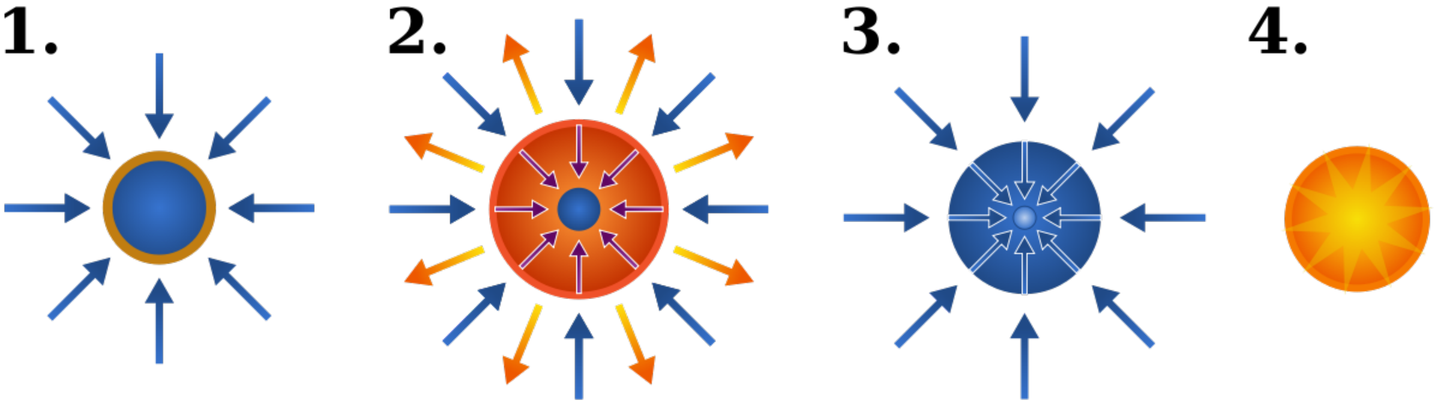


High-fidelity Boundary
Plasma Simulation
SciDAC Project
(PI: CS Chang, PPPL)

Computational methods for Inertial Confinement Fusion

What is Inertial Confinement Fusion?





Radiation hydrodynamics ("rad-hydro"): the workhorse model in ICF

- Simplest form: Euler + radiation transport (gray, multigroup)

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad (1)$$

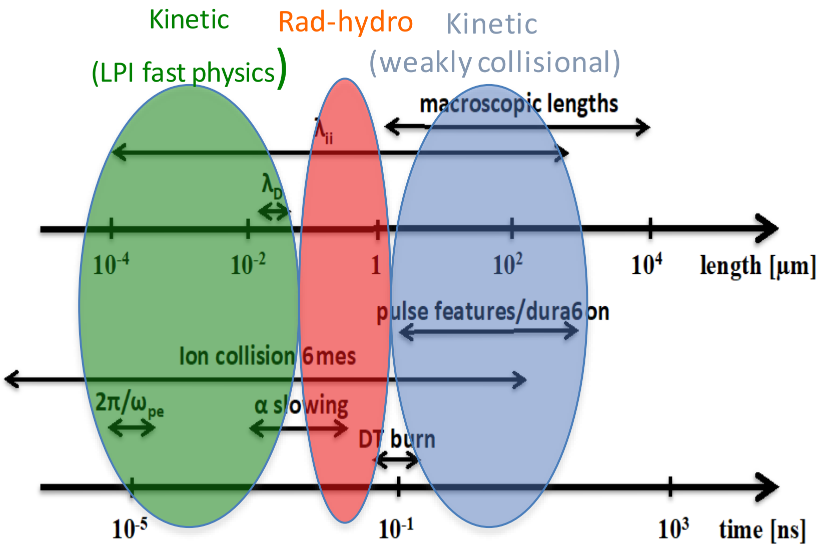
$$\frac{\partial}{\partial t}\rho \mathbf{v} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p = +\rho(\mathbf{a}_{\mathrm{ext}} + \mathbf{a}_{\mathrm{rad}}) \qquad (2)$$

$$\frac{\partial}{\partial t}e + \nabla \cdot [(e + p)\,\mathbf{v}] = +\rho \mathbf{v} \cdot (\mathbf{a}_{\mathrm{ext}} + \mathbf{a}_{\mathrm{rad}}) - \kappa_{\mathrm{P}} \rho c (a_{\mathrm{R}} T^4 - E) \qquad (3)$$

$$\frac{\partial}{\partial t}E + \nabla \cdot \mathbf{F} = \kappa_{\mathrm{P}} \rho c \left(a_{\mathrm{R}} T^4 - E\right). \qquad (4)$$

Radiation hydrodynamics ("rad-hydro"): assumptions and limitations

- Quasineutrality
- Electrostatic limit (magnetic fields ordered out due to large plasma β)
- High collisionality (local thermal equilibrium)
- Single fluid
- Cannot account for multiple species, or deviations from thermal equilibrium

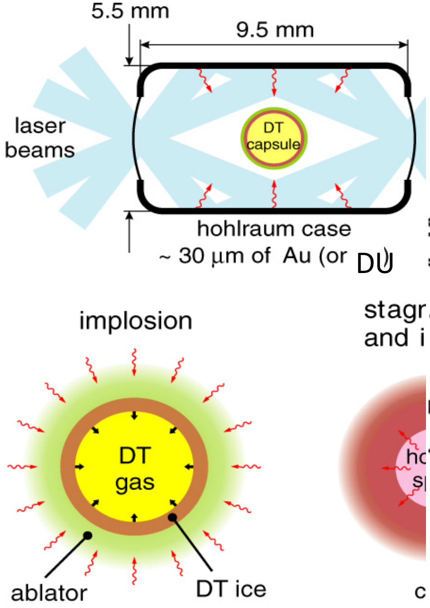


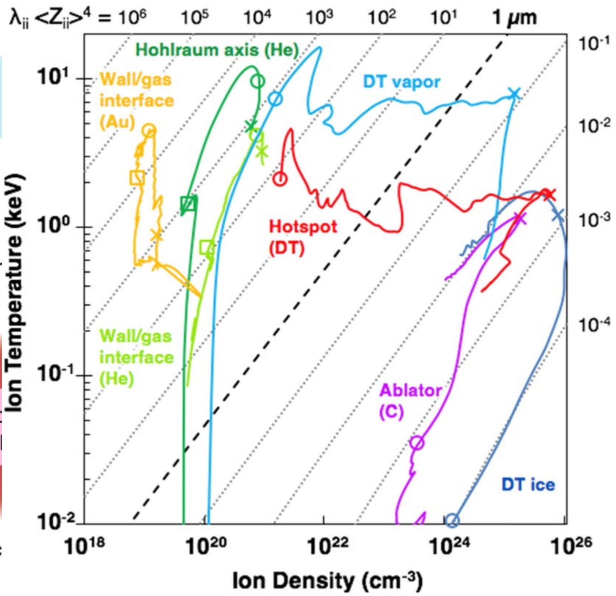
Radiation hydrodynamics (”rad-hydro”): methods

- Spatial discretization:
  - Hydro: Eulerian or Lagrangian (moving mesh)
  - Radiation: Monte Carlo (particles), discrete ordinates (Sn). Typically considers multiple energy groups (i.e., photon frequencies)
- Temporal discretization:
  - Hydro: explicit
  - Radiation (stiff): fully implicit, semi-implicit (some parts implicit, others explicit).
    - Much recent work in multiscale methods (so-called high-order/low-order, HOLO), where moment descriptions (”radiation-diffusion” models) are used to accelerate kinetic solvers.

Beyond rad-hydro: evidence that more fidelity is needed

Post-simulation analysis indicate weakly collisional regimes are present

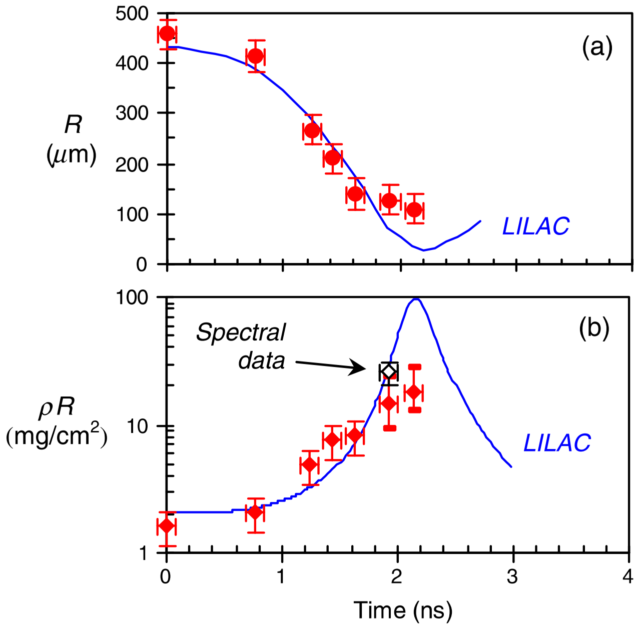




Rinderknecht et al., PPCF (2018)

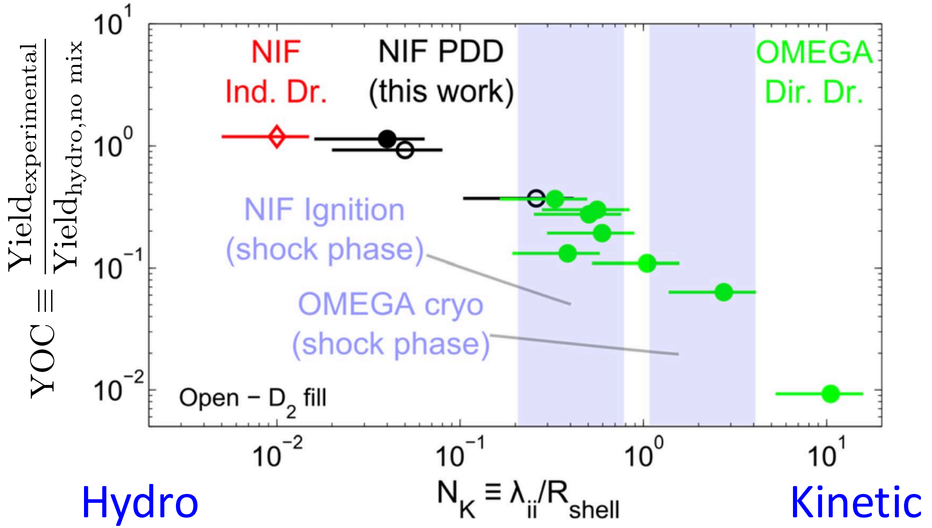
Beyond rad-hydro: evidence that more fidelity is needed

Simulations overpredict compression and yield



20-μm thick CH shell, 15 atm. H_2 fill

Li *et al.*, PRL **100**, 225001 (2008)



Hydro

Kinetic

Rosenberg, PRL (2014)

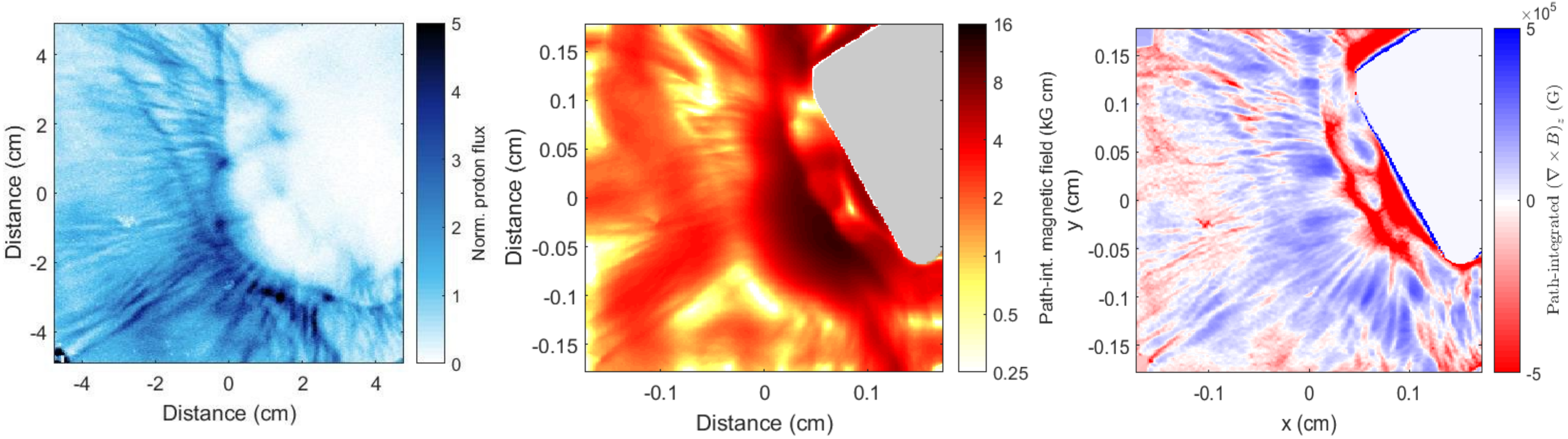
Beyond rad-hydro: evidence that more fidelity is needed

Evidence of importance of electromagnetic effects

Proton radiographs

Path-integrated B fields

MHD current $4\pi c^{-1} J_z = (\nabla\times\mathbf{B})_z$



[1] Li, C. K., et al. "Study Plasma Stagnation in Laser-Driven Hohlraums." *Bulletin of the American Physical Society* 62 (2017).

Beyond rad-hydro: what will it take?

- Presently, 3D-3V VFP+Maxwell solvers are out of reach
- Focus on 1D-2V geometries (planar, spherical symmetry)
- Consider suitable asymptotic limits for Maxwell equations:
  - Electrostatic approximation (exact in 1D spherical, $\beta \sim 10^3$-10^4 in Omega)
  - Quasineutrality: $\rho = \sum q_i n_i = 0$
  - Ambipolarity: $j = \sum q_i n_i v_i = 0$ (in 1D)
  - Eliminates fastest time scales (plasma frequency) and smallest length scales (Debye length)
- Consider fluid electrons:
  - Rigorous fluid model for multiple kinetic ion species, including thermal and friction forces (Simakov et al, PoP 2014)
  - However, it eliminates non-local heat transport effects (important; need kinetic electrons for this)
- Ions remain fully kinetic, allow for multiple species

Taitano et al., CPC **258** (2021); JCP **365** (2018); JCP **318** (2016); JCP **297** (2015)

Model equations: fully kinetic ions + fluid electrons

Vlasov-Fokker-Planck
for ion species

Fluid electrons

$$\frac{3}{2}\partial_t\left(n_e T_e\right) + \frac{5}{2}\partial_x\left(u_e n_e T_e\right) - u_e \partial_x\left(n_e T_e\right) - \partial_x \kappa_e \partial_x T_e = \sum_\alpha C_{e\alpha}$$

$$n_e = -q_e^{-1}\sum^{N_s} q_\alpha n_\alpha \qquad u_e = -q_e^{-1} n_e^{-1} \sum_{\alpha \neq e}^{N_s} q_\alpha n_\alpha u_\alpha$$

Electric field model: e pressure, friction, thermal forces

$$E = -\frac{\nabla p_e + \sum_i \mathbf{F}_{ie}}{e n_e} = -\frac{\nabla p_e}{e n_e} - \frac{\alpha_0(Z_{eff}) m_e}{e}\sum_i \nu_{ei}(\mathbf{V}_e - \mathbf{V}_i) - \frac{\beta_0(Z_{eff})}{e}\nabla T_e$$

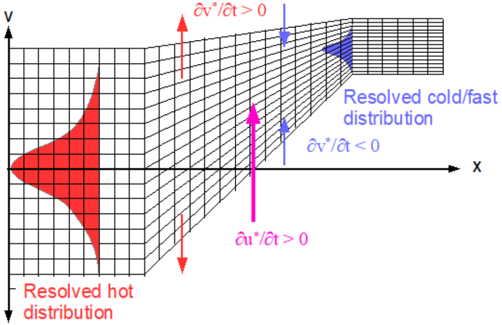
Simakov and Molvig, PoP **21** (2014)

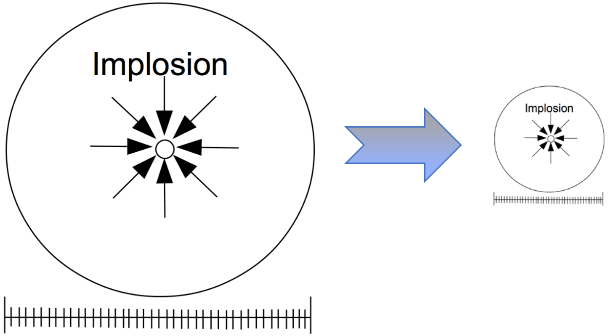
Beyond rad-hydro: naïve algorithms will not work, even with asymptotic models

- Mesh requirements:
  - Intra species $v_{th,max}/v_{th,min} \sim 100$
  - Inter species $(v_{th,\alpha}/v_{th,\beta})_{max} \sim 30$
  - $N_v \sim [10(v_{th,max}/v_{th,min}) \mathrm{x} (v_{th,\alpha}/v_{th,\beta})]^2 \sim 10^9$
  - $N_r \sim 10^3\text{-}10^4$
  - **$N=N_r N_v \sim 10^{12}\text{-}10^{13}$ unknowns in 1D2V!**
- Timestep requirements: $\Delta t_{exp}^{coll} \sim \frac{1}{10}\left(\frac{\Delta v}{v_{th}^{min}}\right)^2 \nu_{coll}^{-1} \sim 10^{-9}\, ns$
  - t_{sim}=10 ns
  - **$N_t=10^{10}$ time steps**
- Beyond exascale (>10^{23} FLOPS)!

Beyond rad-hydro: algorithmic innovation is the solution!

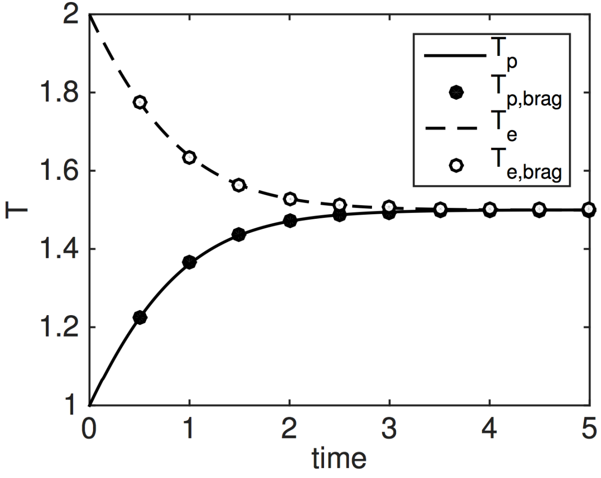
- Fully nonlinearly time-implicit ($\Delta t >> \tau_{col}$)
  - Iterate solution to convergence
  - Use fluid models to accelerate kinetic solution
- Optimal, adaptive grid in phase space
  - Adaptivity in velocity space based on shift and normalization to thermal speed
  - Moving radial mesh in physical space to follow capsule implosion



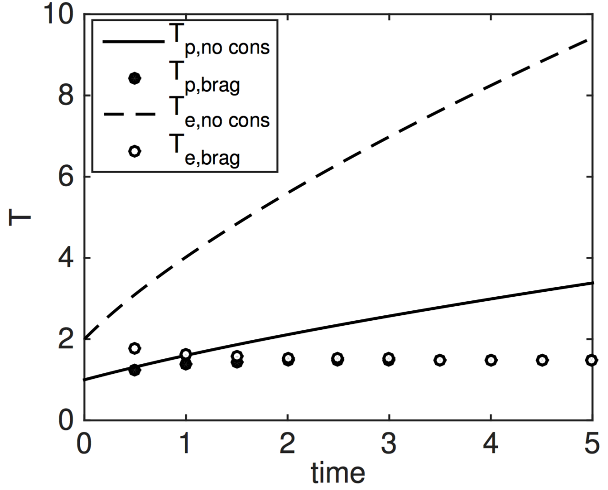


- Fully conservative (mass, momentum, and energy) and asymptotic preserving (able to capture LTE solution in strongly collisional regimes)

Beyond rad-hydro: Why is strict conservation critical?



With energy conservation

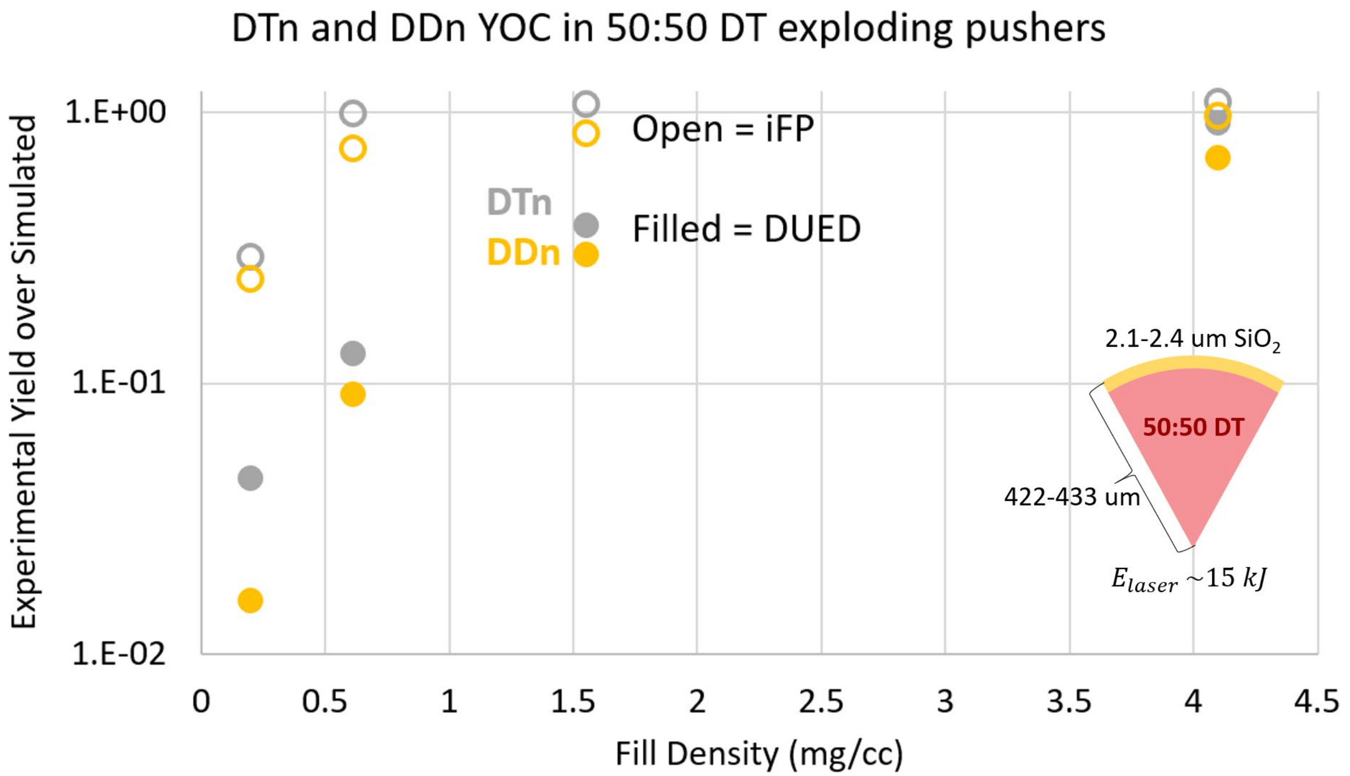


Without energy conservation

Beyond rad-hydro: algorithms enable hybrid VFP-fluid simulations of entire capsule implosions

- Mesh requirements:
  - v-space adaptivity with v_{th} normalization and $u_{||}$ shift, $N_v \sim 10^4$-10^5
  - Moving mesh in physical space, $N_r \sim 10^2$
  - Second-order accurate phase-space discretization
  - **$N=N_v N_r \sim 10^6 \sim 10^7$** (vs. 10^{12} with static mesh)
- Timestep requirements:
  - Optimal $O(N_v)$ implicit nonlinear algorithms
  - Second-order-accurate timestepping
  - $\Delta t_{imp}=\Delta t_{str} \sim 10^{-3}$ ns
  - **$N_t \sim 10^3$-10^4** (vs. 10^{10} with explicit methods)
- Terascale-ready! (10^{12} FLOPS, any reasonable cluster)
  - Currently taking a few hours on 400 cores for full capsule implosion simulations!

Beyond rad-hydro: VFP modeling successfully predicts experimental trends!



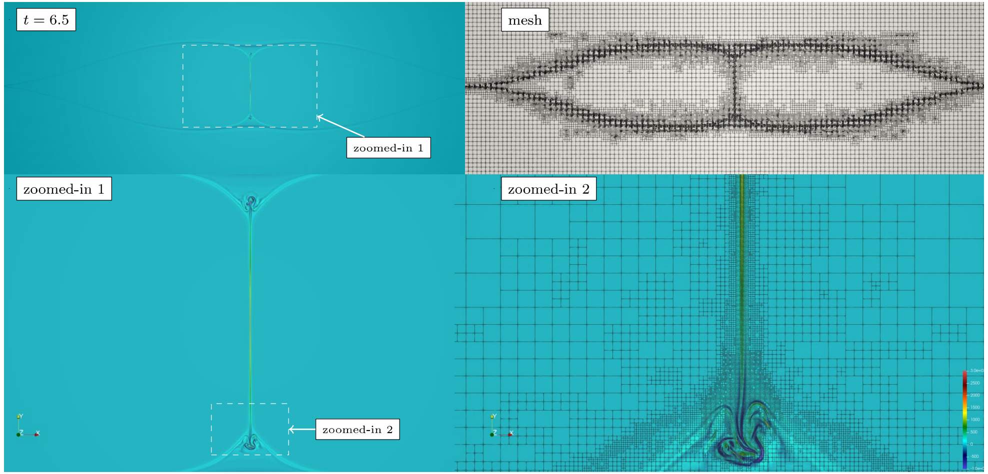
A few examples of future research directions in Fusion Computation

Trends and directions in fusion computation

- There are several drivers of innovation in fusion computation:
  - Drive towards whole-device modeling in ICF and MFE
  - Drive towards higher simulation fidelity via model integration (e.g., MHD+GK, hybrid fluid-kinetic, etc.)
  - Drive towards exascale computing (10^{18} FLOPS!)
- There are many efforts around the world responding to these trends
  - Algorithms remain a key enabling technology for the simulations of the future, in the development of multiscale numerical formulations, spatial discretization and adaptivity, or in temporal integration via advanced (scalable) solvers
- I will comment next on a few directions of particular personal interest. These are just intended as examples, acknowledging that there are as many views on this topic as practitioners in the field.

Towards exascale with fully implicit, adaptive MHD solvers

- We have been exploring the use of MHD physics-based preconditioning in combination with exascale-ready libraries for spatial discretization (MFEM) and solvers (PETSc, Trilinos)
- These libraries offer tremendous flexibility in discretization and solver choices, and offer state-of-the-art adaptive mesh refinement capabilities
- Physics-based preconditioning is discretization agnostic, so can be readily implemented with any discretization strategy.
- We have demonstrated the capability with system-scale simulations of magnetic reconnection using realistic values of resistivity and viscosity



Simulation of island coalescence in 2D with fully implicit solver and AMR in MFEM with $\nu = \eta = 10^{-6}$. Mesh dofs is 0.21% of an equivalent uniform mesh.

Tang et al, JCP, submitted (2021)

Fully implicit GK electromagnetic PIC solvers

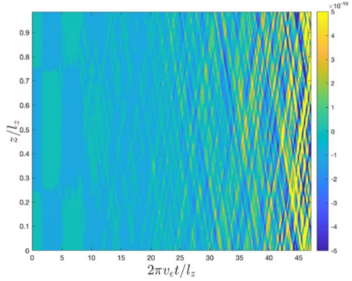
- Semi-implicit GK PIC algorithms are known to suffer from two numerical problems:
  - Cancellation errors: arise from lack of cancellation of skin currents represented on both the mesh and the particles (needed for numerical stability)
  - Finite-grid instabilities: due to aliasing errors arising from particles living in the continuum, while fields live on a discrete mesh
- Both these issues can be eliminated with fully implicit methods

Sturdevant et al., PoP, accepted (2021)
Sturdevant el al., JCP, submitted (2021)

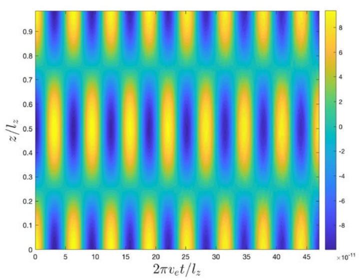
Fully implicit algorithms in XGC

	# iterations		
β_e in %	$\frac{v_{te}\Delta t}{R_0\Delta\varphi}=0.25$	$\frac{v_{te}\Delta t}{R_0\Delta\varphi}=1.00$	$\frac{v_{te}\Delta t}{R_0\Delta\varphi}=4.00$
0.5	3.9	5.0	5.5
7.7	5.0	6.2	7.1
23.1	5.9	7.0	8.3

β_e in %	$\frac{v_A\Delta t}{R_0\Delta\varphi}$	# iterations
2.8×10^{-2}	0.1	3.3
2.8×10^{-4}	1.0	4.0
2.8×10^{-6}	10.0	4.0



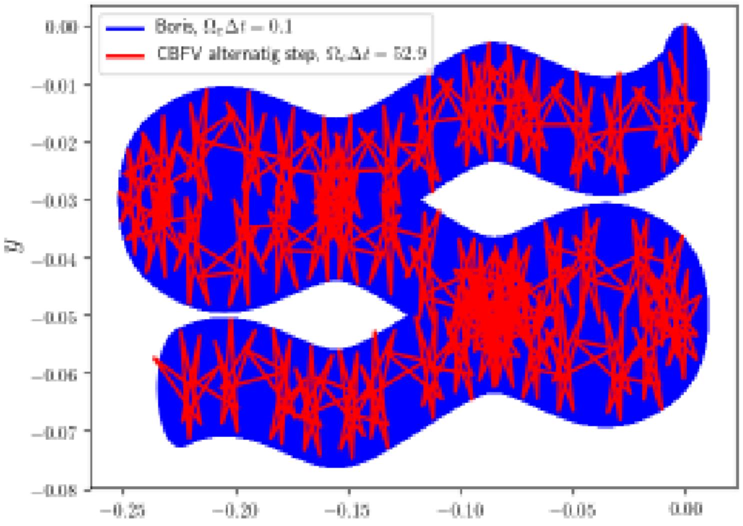
Unstable



Stable

Toward 6D simulations of MFE devices

- GK model has limitations due to asymptotic approximations:
  - Break down in the presence of strong plasma gradients, such as in high-confinement conditions (due to pressure pedestal)
- Improving fidelity with require multiscale numerical representations that can seamlessly transition between GK and full descriptions (5D to 6D and back; asymptotic-preserving).



Ricketson et al, JCP (2020)

- This will demand specialized algorithms and solvers
  - Fully implicit timestepping with strong conservation properties (for stability and accuracy)
  - Asymptotic-preserving particle orbit integrators that capture orbit without following gyromotion
  - Use of nested model hierarchy for full algorithmic acceleration (e.g, use MHD to accelerate a fully kinetic simulation).

Multi-D hybrid kinetic/fluid modeling of ICF hohlraums

- Hohlraums perform critical energy conversion process from laser to X-rays
- Hohlraum environment is rarefied (or vacuum) ⇒ kinetic effects are important, cannot be modelled with rad-hydro
  - Plasma expansion into vacuum
  - Multiple ion species
  - Beam interpenetration
- Large electromagnetic fields have been measured in hohlraums, cannot be neglected
- Hohlraum modeling uncertainty is preventing progress in ICF implosion optimization towards ignition

Rad-hydro	Our approach
High-collisionality (fluid)	Arbitrary collisionality (kinetic)
Single quasi-neutral fluid, no B field	Multiple ion kinetic species Fluid electrons + HOT electrons Fully electromagnetic
Linear LPI	Nonlinear LPI
Radiation transport (IMC, Sn)	Radiation transport (HOLO-DP)
LTE and NLTE atomic physics	
Laser ray tracing (Mazinisin, in collaboration with LLE)	

- At LANL, we have started developing the first multi-D hybrid kinetic ion/fluid electron code for hohlraum modeling.

Summary

Summary

- Thermonuclear fusion poses great challenges to the computational physicist
- Challenges have been met by ingenuity in developing an asymptotic model hierarchy, as well as solvers and algorithms
- Fusion has been a pioneer in HPC, driving the creation of the first unclassified computer systems (now NERSC)
- Fusion has also driven significant algorithmic innovation, and has been a pioneer in the use of modern discretizations and implicit timestepping schemes.
- Both MFE and ICF are pushing the computational frontier towards higher fidelity (kinetic) simulations, by leveraging model nesting, scalable solvers, and smart algorithms.
- These computational capabilities will continue to inform future iterations of “virtual experiments”, with the goal of harnessing fusion energy on Earth.