Unifying Modeling Of Tokamak Plasmas

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Introduction: This white paper first highlights new 3-D issues emerging from present tokamak experiments and boundary issues that need to be included in integrated simulations of present and ITER plasmas. Then, self-consistent unification [1,2] of the currently mostly independent tokamak magnetohydrodynamic (MHD), kinetic and transport models and simulation codes via a Chapman-Enskog-based framework is presented. The vision here focuses on: what new physical effects should be included?, what equations need to be solved?, and how can they be unified in a self-consistent framework? This white paper's thesis is that a fluid-based, comprehensive modular approach that unifies extended MHD, kinetics via a Chapman-Enskog approach, and transport analyses using a combination of analytic studies and simulations needs to be developed and implemented.

New tokamak plasma issues: It has become increasingly clear recently that the effects and evolution of the toroidal plasma flow in small gyroradius tokamak plasmas with diamagnetic-level flows needs to be taken into account — in extended MHD modeling of the magnetic field structure and simultaneously with density and temperature transport. This is especially true for plasma responses to small 3-D magnetic fields [3] (field errors, NTV, RMPs, NTMs etc.) that can lead to locked-mode disruptions, and in the near-separatrix edge region (pedestals [4], ion orbit losses, charge-exchange, RMP effects [5-7], radial electric field etc.). Further, addressing boundary plasma issues (pedestals, SOLs, divertor region and plasma-material interactions) has been identified recently [8] as a major new programmatic thrust for the magnetic fusion program. Also, the interactions of 3-D and boundary effects with the core plasma's disruptivity, **B** field structure and transport evolution are becoming increasingly important and problematic.Thus, the present challenge for integrated simulations of tokamak plasmas is to move beyond its present primary focus on core (and recently pedestal) plasma stability and microturbulence-driven transport in mostly axisymmetric equilibrium models to encompass small 3-D **B** field effects and boundary plasmas in a self-consistent framework that facilitates modeling of modern tokamak plasmas.

Plasma species equations: The fundamental plasma kinetic equation (PKE) for the six-dimensional (6-D, $\mathbf{x}, \mathbf{v}$) distribution function $f(\mathbf{x}, \mathbf{v}, t)$ of a plasma species s in a tokamak is given by $df/dt = \mathcal{C}\{f\} + \mathcal{S}\{f\}$. Here, $df/dt \equiv \partial f/\partial t + \mathbf{v} \cdot \partial f/\partial \mathbf{x} + (q/m)[\mathbf{E} + \mathbf{v} \times \mathbf{B}] \cdot \partial f/\partial \mathbf{v}$ is the Vlasov operator, $\mathcal{C}\{f\}$ is the Fokker-Planck Coulomb collision operator and $\mathcal{S}\{f\}$ is a source operator that represents the long, transport time scale effects of various sources (e.g., neutral beam and wave heating, current-drive) and sinks (e.g., radiation, edge charge-exchange). While this plasma kinetic equation is fundamental, for times longer than species collision times (i.e., $t > 1/\nu_s$), 3-D ($\mathbf{x}$) fluid equations (for extended MHD and transport) are feasible, appropriate, useful and needed for modeling present and ITER tokamak plasmas. The $\int d^3v\,(1, m\mathbf{v}, mv^2/2)$ moments of the PKE yield complete species fluid moment equations [1,9] for the density n, flow velocity $\mathbf{V}$ and pressure $p \equiv nT$ or entropy $s_{\rm M} \equiv (3/2)\ln(p/n^{5/3})$ of each species. The resultant species fluid equations are exact to the extent that relevant closure moments can be obtained for the stress tensor $\boldsymbol{\pi}$, heat flux $\mathbf{q}$, and Coulomb collision-induced friction force $\mathbf{R}$ and energy exchange between species Q. Complete fluid equations [1,9] include the sources and sinks of density S_n, momentum $\mathbf{S_p}$ and energy $S_{\mathcal{E}}$.

Chapman-Enskog approach: The Chapman-Enskog Ansatz [10] posits that the species distribution has two parts — a "dynamic" space- and time-dependent Maxwellian $f_{\rm M}$ plus kinetic distortion F: $f(\mathbf{x}, \mathbf{v}, t) = f_{\rm M}(\mathbf{x}, \mathbf{v}, t) + F(\mathbf{x}, \mathbf{v}, t)$, in which $f_{\rm M}(\mathbf{x}, \mathbf{v}, t) \equiv \frac{n(\mathbf{x},t)}{[2\pi\, T(\mathbf{x},t)/m]^{3/2}}\, e^{-m\,|\mathbf{v}_r|^2/2T(\mathbf{x},t)}$ where $\mathbf{v}_r \equiv \mathbf{v} - \mathbf{V}(\mathbf{x}, \mathbf{v}, t)$. The kinetic distortion F is not assumed to be small and can have velocity-space loss cones, e.g., near the separatrix. Substituting this Ansatz into the PKE yields the general Chapman-Enskog kinetic equation (CEKE) $dF/dt - \mathcal{C}\{f\} - \mathcal{S}\{f\} = -\,df_{\rm M}/dt$ [1,11]. After using the species fluid equations, $df_{\rm M}/dt$ indicates the inhomogeneous "drives" for F are caused by ∇T, flow-induced strains ($\mathsf{W} \sim \nabla \mathbf{V}$), closures $\boldsymbol{\pi}$, $\mathbf{R}$, and sources $S_n, \mathbf{S_p}$, entropy $\dot{s}_{\rm M}$. When collisions dominate, the solution of this CEKE produces [1] closures for $\boldsymbol{\pi}, \mathbf{q}, \mathbf{R}, Q$ that yield the Braginskii collisional fluid equations [12]. Solutions in 1-D yield the collisionless nonlocal heat flux closure [13] and general collisionality closures [14,15]. The Chapman-Enskog formalism was introduced initially for linear drift wave instabilities in a sheared slab magnetic field [16,17] and neoclassical processes [18]. Its general form [1,11] includes collisional effects and is more complete [1,19] for developing kinetic/fluid models than the δf approach [20,21] or gyrofluid closures [22,23].

Fundamental approximations: Tokamak plasmas have collision frequencies ν_s much smaller than charged particle gyrofrequencies ω_{cs} and thermal gyroradii $\varrho_s \equiv v_{Ts}/\omega_{cs}$ small compared to equilibrium scale lengths. Thus, they are magnetized plasmas in which a small gyroradius approximation is appropriate: $\varrho_* \equiv \varrho_i|\nabla \ln(\mathbf{B}, n, T)| \sim \varrho_i/L \ll 1$. Its physical consequences are: ϱ_*^0 ($\sim \mu$s) particle guiding center motion along $\mathbf{B}$, Alfvén and sound waves, radial force balance equilibrium, poloidal flux surfaces $\psi_{\rm p}$; ϱ_*^1 ($\sim$ ms) particle drifts $\perp$ to $\mathbf{B}$, flows within flux surfaces, collision-induced magnetic reconnection at rational surfaces where $q = m/n$; and ϱ_*^2 ($\sim$ s) plasma transport across flux surfaces induced by collisions and microturbulence, and 3-D field effects. Thus, the closure and collisional moments $\boldsymbol{\pi}, \mathbf{q}, \mathbf{R}$ are all highly anisotropic and different along $\mathbf{B}$ ($\|, \varrho_*^0, \sim \mu$s), perpendicular to $\mathbf{B}$ ($\wedge, \varrho_*^1, \sim$ ms) and across ψ_p flux surfaces ($\perp, \varrho_*^2, \sim$ s).

Extended MHD: Summing fluid equations over species yields extended MHD equations [1,24]. Tokamak plasmas are quasineutral ($\nabla \cdot \mathbf{J} = -\partial \rho_q/\partial t \simeq 0$). The magnetic field $\mathbf{B}$ in them is determined from the pre-Maxwell equations $\partial \mathbf{B}/\partial t = -\nabla \times \mathbf{E}$, $\nabla \cdot \mathbf{B} = 0$, and current density $\mathbf{J}$ from $\mathbf{J} = \nabla \times \mathbf{B}/\mu_0$. Extended MHD equilibrium (of compressional Alfvén waves, when $t > \bar{a}/c_{\rm A} \sim \mu$s) yields the plasma radial force balance and Grad-Shafranov equation for $\psi_{\rm p}$. The $\nabla \psi_{\rm p} \cdot$ component of its two-fluid Ohm's law [24] yields a relation between $\mathbf{E} \times \mathbf{B}$, diamagnetic, and toroidal, poloidal flows within a flux surface: $\Omega_{\rm tor} \equiv \mathbf{V}_i \cdot \nabla \zeta = -[d\Phi_0/d\psi_{\rm p} + (1/n_i q_i)(dp_i/d\psi_{\rm p})] + q\mathbf{V}_i \cdot \nabla \theta$. The M3D-C1 [25] and NIMROD [26] extended MHD codes also check for macrostability (both ideal and tearing-type), and when stress closures are included can solve for order ρ_* flows and the evolving $\mathbf{B}$ field in the plasma responses to 3-D fields and in reconnection regions with limited flow screening.

Chapman-Enskog kinetics: Since by construction $\int d^3v\,(1, \mathbf{v}_r, v_r^2)\,F = 0$, solutions of the CEKE for F will not produce extraneous δn, $\delta \mathbf{V}$, δp or $\delta \mathbf{J}$ terms; hence closures obtained from them will be consistent with species fluid equations. Thus, the CEKE approach automatically embodies extended MHD, order ρ_* flows and the evolving $\mathbf{B}$ field, and produces as "output" extended MHD closures and complete radial transport fluxes that include small 3-D $\mathbf{B}$ field and boundary effects. Rigorous drift-kinetic CEKEs have been derived [27,28] and are being solved numerically for axisymmetric tokamaks [29,30]. Gyrokinetic versions of the Vlasov equation [31] and PKE [32] have been developed, but are not consistent with extended MHD [24] or the transport equations in [36-38]. A gyrokinetic CEKE needs to be worked out and used to determine transport fluxes caused by 3-D $\mathbf{B}$ fields and boundary effects in conjunction with those induced by collisions and microturbulence.

Transport equations: The ONETWO [33], TRANSP [34] and ASTRA [35] 1-1/2 D transport codes are based on adaptations of the inapplicable and incomplete [1] Braginskii [12] collisional transport equations. Complete tokamak core plasma transport equations [36] have been derived [37,38]. These equations need to be solved for the plasma toroidal angular momentum density $L_{\rm tor} \equiv \rho_m \langle R^2 \rangle \Omega_{\rm tor}$ (hence radial electric field) along with electron density, and electron and ion pressures. Outside the separatrix the present [4] 2-D SOLPS [39] and UEDGE [40], and 3-D EMC3-EIRENE [41–43] boundary codes use truncated versions of the inapplicable Braginskii equations. In the semi-collisional boundary region CEKE-based closures are needed to include kinetic effects.

Summary: The opportunity, gap and need is to adopt a modular approach for developing and iteratively solving the fluid model extended MHD and transport equations using Chapman-Enskog kinetic solutions for closures as the framework for integrated simulations of tokamak plasmas.

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[9] The complete fluid moment equations for a given species s in a tokamak plasma are [1]:

$$\text{density} \qquad (\partial/\partial t + \mathbf{V}_s\cdot\boldsymbol{\nabla})\, n_s = -\, n_s \boldsymbol{\nabla}\cdot\mathbf{V}_s + S_{n\,s}, \tag{1}$$

$$\text{momentum} \qquad m_s n_s\, (\partial/\partial t + \mathbf{V}_s\cdot\boldsymbol{\nabla})\, \mathbf{V}_s = n_s q_s\, (\mathbf{E} + \mathbf{V}_s\times\mathbf{B}) - \boldsymbol{\nabla} p_s - \boldsymbol{\nabla}\cdot\boldsymbol{\pi}_s + \mathbf{R}_s + \mathbf{S}_{\mathbf{p}\,s}\,, \tag{2}$$

$$\text{energy} \qquad (3/2)(\partial/\partial t + \mathbf{V}_s\cdot\boldsymbol{\nabla})\, p_s = (5/2)\, p_s \boldsymbol{\nabla}\cdot\mathbf{V}_s + p_s\, \dot{s}_{\mathrm{M}s}, \quad \text{or}, \tag{3}$$

$$\text{entropy} \qquad (\partial/\partial t + \mathbf{V}_s\cdot\boldsymbol{\nabla})\, s_{\mathrm{M}s} = \dot{s}_{\mathrm{M}s} \equiv (-\boldsymbol{\nabla}\cdot\mathbf{q}_s - \boldsymbol{\pi}_s:\boldsymbol{\nabla}\mathbf{V}_s + Q_s + S_{\mathcal{E}\,s})/p_s. \tag{4}$$

Here, n_s, $\mathbf{V}_s$, $p_s \equiv n_s T_s$, $s_{\mathrm{M}\,s} \equiv (3/2)\ln(p_s/n_s^{5/3})$ are the species density, flow velocity, isotopic pressure, collisional entropy and $S_{n\,s}, \mathbf{S}_{\mathbf{p}\,s}, S_{\mathcal{E}\,s}$ are sources and sinks of density, momentum, energy.

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$$\frac{dF}{dt} - \mathcal{C}\{f\} - \mathcal{S}\{f\} = -\frac{df_{\rm M}}{dt}, \qquad \text{general Chapman-Enskog kinetic equation,} \tag{5}$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\left[\mathbf{E} + \mathbf{v}\times\mathbf{B}\right]\cdot\frac{\partial F}{\partial \mathbf{v}}, \qquad \text{Vlasov operator on } F, \tag{6}$$

$$\begin{aligned} \frac{df_{\rm M}}{dt} = f_{\rm M}\Bigg[& \left(\frac{mv_r^2}{2T} - \frac{5}{2}\right)\frac{1}{T}\,\mathbf{v}_r\cdot\boldsymbol{\nabla}T, && T \text{ gradient drive,} \\ & + \frac{m}{T}\left(\mathbf{v}_r\mathbf{v}_r - \frac{v_r^2}{3}\mathsf{I}\right):\mathsf{W}, && \text{rate of strain drive,} \\ & + \frac{1}{p}\,\mathbf{v}_r\cdot(-\boldsymbol{\nabla}\cdot\boldsymbol{\pi} + \mathbf{R} + \mathbf{S}_{\mathbf{p}}) && \text{dissipative force effects,} \\ & + \frac{S_n}{n} + \left(\frac{mv_r^2}{2T} - \frac{3}{2}\right)\left(\frac{2\,\dot{s}_{\rm M}}{3\,p} - \frac{S_n}{n}\right)\Bigg] && \text{transport sources.} \end{aligned} \tag{7}$$

The rate of strain induced by the flow velocity $\mathbf{V}$ is $\mathsf{W} \equiv \frac{1}{2}[\boldsymbol{\nabla}\mathbf{V} + (\boldsymbol{\nabla}\mathbf{V})^{\mathsf{T}} - \frac{2}{3}\mathsf{I}\,\boldsymbol{\nabla}\cdot\mathbf{V}]$.

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$$\begin{aligned}
&\text{mass density} && (\partial/\partial t + \mathbf{V}\cdot\boldsymbol{\nabla})\,\rho_m = -\,\rho_m \boldsymbol{\nabla}\cdot\mathbf{V}, && (8)\\
&\text{charge continuity} && \boldsymbol{\nabla}\cdot\mathbf{J} = 0, && (9)\\
&\text{momentum} && \rho_m(\partial/\partial t + \mathbf{V}\cdot\boldsymbol{\nabla})\mathbf{V} = \mathbf{J}\times\mathbf{B} - \boldsymbol{\nabla}P - \boldsymbol{\nabla}\cdot\mathbf{\Pi}, && (10)\\
&\text{Ohm's law } (t > 1/\nu_e) && \mathbf{E} = -\,\mathbf{V}\times\mathbf{B} + \mathbf{R}_e/n_e e + (\mathbf{J}\times\mathbf{B} - \boldsymbol{\nabla}p_e - \boldsymbol{\nabla}\cdot\boldsymbol{\pi}_e)/n_e e, && (11)\\
&\text{equation of state} && (\partial/\partial t + \mathbf{V}\cdot\boldsymbol{\nabla})\ln(P/\rho_m^{5/3}) = \textstyle\sum_s \dot{s}_{\mathrm{M}s}. && (12)
\end{aligned}$$

The ideal two-fluid MHD equations are obtained by setting all the dissipative terms to zero, i.e., $\mathbf{R}_e$, $\mathbf{\Pi}$, $\boldsymbol{\pi}_e$, $\sum_s \dot{s}_{\mathrm{M}s} \to 0$. The usual ideal MHD equations which neglect diamagnetic flow effects are obtained from these two-fluid ideal MHD equations by neglecting the Hall term using the equilibrium force balance $\mathbf{J}\times\mathbf{B} = \boldsymbol{\nabla}P$ in the two-fluid Ohm's law so that it is simply $\mathbf{E} = -\mathbf{V}\times\mathbf{B}$.

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$$\text{density} \qquad \frac{1}{V'} \frac{\partial}{\partial t}\bigg|_{\psi_{\rm p}} n_e V' + \dot{\rho}_{\psi_{\rm p}} \frac{\partial n_e}{\partial \rho} + \frac{1}{V'} \frac{\partial}{\partial \rho}(V' \Gamma) = \langle \overline{S}_n \rangle, \tag{13}$$

$$\text{tor. mom.} \qquad \frac{1}{V'} \frac{\partial}{\partial t}\bigg|_{\psi_{\rm p}} L_{\rm tor} V' + \dot{\rho}_{\psi_{\rm p}} \frac{\partial L_{\rm tor}}{\partial \rho} + \frac{1}{V'} \frac{\partial}{\partial \rho}(V' \overline{\Pi}_{\rho\zeta}) = \langle \mathbf{e}_\zeta \cdot (\overline{\mathbf{J}\times\mathbf{B}} - \boldsymbol{\nabla} \cdot \overline{\boldsymbol{\Pi}} + \overline{\mathbf{S}}_{\mathbf{p}}) \rangle, \tag{14}$$

$$\text{energy} \qquad \frac{3}{2} p_s \frac{\partial}{\partial t}\bigg|_{\psi_{\rm p}} \ln p_s V'^{5/3} + \frac{3}{2} \dot{\rho}_{\psi_{\rm p}} \frac{\partial p_s}{\partial \rho} + \frac{1}{V'} \frac{\partial}{\partial \rho}(V' \Upsilon_s) + \langle \boldsymbol{\nabla} \cdot \mathbf{q}^{\rm pc}_{*s} \rangle = \overline{Q}_{{\rm net}\, s}, \tag{15}$$

$$\text{poloidal flux} \qquad \frac{\partial \psi_{\rm p}}{\partial t}\bigg|_{\psi_{\rm t}} = D_\eta \, \Delta^+ \psi_{\rm p} - S_{\psi_{\rm p}}, \quad D_\eta \equiv \frac{\eta_\parallel^{\rm nc}}{\mu_0}, \quad S_{\psi_{\rm p}} = \frac{\partial \Psi_{\rm p}}{\partial t} + \frac{\eta_\parallel^{\rm nc}}{I \langle R^{-2} \rangle} \langle \mathbf{B}_0 \cdot \mathbf{J}_{\rm drives} \rangle. \tag{16}$$

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