Kinetic simulation of heat pulse propagation through the tokamak scrape-off layer

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Motivation: Prediction of particle and heat fluxes in future magnetic fusion devices such as ITER

- The PSI SciDAC is developing coupled models for the dynamic interaction between plasma & material surfaces at the edge of a magnetically confined fusion energy reactor

- Our goals are to
  - Determine importance of ELMs on impurity production & material erosion
  - Understand dynamic recycling during transient events

**Plasma**
- $d \sim 10^{-1} - 100 \, \text{m}$
- $\tau \sim 10^{-7} - 10^{-3} \, \text{s}$

**Sheath**
- $d \sim 10^{-5} - 10^{-3} \, \text{m}$
- $\tau \sim 10^{-12} - 10^{-10} \, \text{s}$

**Material**
- $d \sim 10^{-10} - 10^{-6} \, \text{m}$
- $\tau \sim 10^{-12} - 10^{-6} \, \text{s}$
Goal: Simulate heat pulse propagation through the scrape-off layer (SOL) edge plasma

- Goal: Determine the erosion rate of material surfaces that are impacted by large transient events such as edge localized modes (ELMs)

- Study the transient behavior of a heat pulse as it travels along a flux tube using the 4D drift-kinetic COGENT code
  - Results will be benchmarked against heat pulse test problems that have been used to compare physics models and numerical algorithms

- An important goal will be to determine under what conditions energetic particle tails are found to form and whether kinetic effects impact quantitative results
Plan: develop 4D COGENT model for ELM-relevant simulation of transient heat loads

- Develop a 4D COGENT model for simulation of transient heat loads relevant to edge-localized mode instabilities (ELMs)
  - Implement ELM-relevant heat pulse model within the COGENT code in simplified geometry & perform verification studies
  - Predict the plasma fluxes impinging on the sheath
  - Compare heat pulse simulations to fluid models and experimental data
  - Develop models for nonlinear sheath BCs & for accurately exchanging data with sheath code

- As new capabilities are developed jointly with the ESL team & AToM-SciDAC, we will develop new capabilities
  - Unlike species collisions: electron-ion
  - Neutral physics models including ionization, charge-exchange, radiation
  - Implicit treatment of both collisionless and collisional kinetic transport
  - 5D simulation of drift-kinetic plasma instabilities
Overview of COGENT

• **COGENT is a full-\(F\) continuum gyrokinetic (GK) code**
  - Multi-species gyro-kinetic equations and gyro-Poisson field equations
  - Fokker-Planck collision operators
  - At present, the code handles the long-wavelength drift-kinetic regime \(k_\rho<<1\), but extension to short wavelength is planned for the future
  - Reduced physics models are also available: model collision operators, vorticity equation, fluid electrons, etc.

• **To date, the main research thrust has been focused on obtaining axisymmetric solutions in realistic tokamak geometry, in isolation from wall physics**
  - A non-axisymmetric (5D) version of the code has recently become operational and has been successfully verified in the simulations of the collisionless drift (universal) instability in simplified slab geometry

• **We will focus on improving the capabilities necessary for modeling plasma-wall interactions in the divertor region**
The COGENT team includes both physics & math developers

- COGENT is part of the Edge Simulation Laboratory (ESL), the integrated modeling (AToM) SciDAC, and the PSI SciDAC
  \- ESL: FES physics team at LLNL & ASCR applied math team at LBNL & LLNL

- Algorithmic Capabilities
  - 4th Order Finite Volume Discretization and interpolation
    \- Discretization errors are bounded, even near the X-point of a separatrix
  - Mapped multiblock grid technology
    \- Flux surfaces in different topological regions are mapped from the physical toroidal geometry onto topologically rectangular grid blocks
    \- High-order interpolation is used to provide data communication in the region where grid blocks overlap, e.g. near the X-point
  - Implicit algorithms & IMEX capability
    \- IMEX capability has been successfully used to treat the Fokker-Planck collision operator implicitly for like-species collisions
    \- Improves simulation efficiency well into the collisional regime, a regime that is notoriously difficult to treat using kinetic codes
Example: COGENT has recently obtained self-consistent results for the tokamak pedestal*

- Results of an axisymmetric (4D) COGENT simulation of cross-separatrix plasma transport in a DIII-D discharge using full Fokker-Plank ion-ion collisions and self-consistent 2D electrostatic potential variations with the reduced vorticity model for isothermal electrons.

ELM Benchmark (*): determine heat flux due to ELMs for JET-like pedestal parameters

- **JET-like SOL parameters**
  - $B_t = 3$ T, $R = 3$ m, $L_{pol} = 8.3$ m
  - angle $= 6^\circ$, $B_p/B_t = 0.11$
  - $2 L_{\parallel} = 80$ m, $L_{src} = 25$ m
  - $m_i = 2 m_p$
  - $n_{ped} = 5 \times 10^{19}$ m$^3$
  - $T_{ped} = 1.5$ keV
  - $C_{s,ped} = 3.8 \times 10^5$ m/s

- **Maxwellian Source**
  - Source parameters are set to the pedestal parameters (A=1.2)

$$S = \frac{S_{src}}{(2\pi T_{src}^3)^{1/2}} e^{-(mv^2/2+\mu B)/T_{src}} \quad S_{src} = An_{ped} C_{s,ped}/L_{src}$$

- **(*) References**
We can develop understanding using kinetic ions and an adiabatic electron model

- **Collisionless kinetic ion model**

- **Adiabatic = Boltzmann electron model (fixed $T_e$)**

  \[ e\varphi = e\varphi_{sheath} + T_e \log(n_i/n_0) \quad e\varphi_{sheath} = \frac{1}{2}T_e \log\left(V_{i\parallel}^2 m_e/2\pi T_e\right) \]

- **Heat flux at target plate (Assume $T_e = T_i$ at target plate)**

  \[ Q_i = Q_{i,\text{conv}} + Q_{i,\text{cond}} + Q_{i,\text{sheath}} \quad Q_{tot} = Q_i + Q_e \]

  \[ Q_{i,\text{conv}} = \frac{3}{2}T_i \Gamma_i \]

  \[ Q_{i,\text{sheath}} = e\varphi_{sheath} \Gamma_i \]

  \[ Q_e = 2T_e \Gamma_i \]
COGENT results: The heat is on!

- **Parameters for these cases**
  - Resolution: $R \times Z = 8 \times 32$, $\nu \times \mu = 32 \times 32$
  - $n_{SO} = 2 \times 10^{19} \text{ m}^3$
  - $T_{SO} = 175 \text{ eV}$, $T_{e}=210 \text{ eV}$
  - $T_{sr} = 1500 \text{ eV}$
  - $S_{sr} = 9 \times 10^{23} / \text{sm}^3$
COGENT results: $\tau_{ELM} = 200\mu$s

Moments

- $T_{up}$ rises to 1 keV
- $T_{dn}$ rises to 0.9 keV
- Heat flux $Q_{||}=5$ HW/m² peaks after $\tau_{ELM}$
- Temperature profile inverts after $\tau_{ELM}$
COGENT results: $\tau_{ELM} = 200\mu$s

Particle distribution function

- PDF is not Maxwellian
  - Sonic outflows at target plates
  - $T_{\parallel} < T_{\perp} = 1.5$keV at midplane
  - Transition to $\frac{1}{2}$ Maxwellian in $v_{\parallel}$ near target plates
Dependence of maximum heat flux on $\tau_{\text{ELM}}$ is sublinear

- Maximum heat flux achieved $\sim \tau_{||} = 60$ µs after $\tau_{\text{ELM}}$

- Magnitude of heat flux $Q_{||}$ has a power law dependence on $\tau_{\text{ELM}}$ with exponent $< 1$
We are working towards simulations with 2 kinetic species: electrons and ions

• Example: Solution with a self-consistent sheath

• Results of a simulation of the sheath using kinetic electrons with BGK collisions, kinetic hydrogen and a full 2D electrostatic potential model
  – Resolution: 8X x 48Y x 32V|| x 24µ

• Low density $n_e \sim 2 \times 10^{16}/m^3$ allows one to resolve the sheath $\lambda_d = 0.2$ mm in a domain of 1 cm length for temperature $T_e \sim 13.5$ eV, $T_i = 4.5$ eV
Implementation of “gyrokinetic sheath” BCs* allows for efficient quasineutral simulation of a large domain

- **Gyrokinetic Poisson:** retain polarization current but eliminate vacuum polarization

- **“Sheath BC”** = electrons reflected if \(m_e v_\parallel^2/2 < \phi\) in last grid cell in domain before boundary

- **Parameters:**
  
  \[8 R \times 16 Z \times 32 v_{\|} \times 24 \mu\]

  \(n_{\text{init}} = 10^{19} \text{ m}^{-3}\)

  \(T_{\text{init}} = 100 \text{ eV}\)

  \(m_e/m_i = 0.01\)

  Snapshot at \(t = 3 \mu\text{s}\)

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Future Work: explore the importance of kinetic plasma effects

- Kinetic effects have the potential to strongly impact surface evolution
  - Heat fluxes are strongly flux-limited during the early phase of an ELM
  - Energetic ions can alter the
    - ion saturation current
    - charge exchange rate
    - rates for implantation, sputtering, and defect formation
  - Energetic electrons can alter the
    - heat flux directed on PFCs
    - sheath potential which determines ion energy on impact
    - rates for threshold processes such as ionization, recombination, and radiation
  - It is known that kinetic effects alters the quantitative ratio of electron to ion heat flux 1:1 vs. 3:1 (Havlikova PPCF 2012)

- Kinetic processes are potentially important for interpretation of experimental data and for validation exercises
  - Non-Maxwellian distributions can change the interpretation of standard diagnostic techniques based on Langmuir probes and impurity radiation
Conclusions

• PSI SciDAC is developing dynamically coupled plasma-wall models
  – Ultimate goal is to determine the erosion rate of material surfaces that are impacted by large transient events such as ELMs

• ELM heat pulse benchmark has been simulated using an adiabatic Boltzmann electron model
  – Results appear to match reasonably well
  – Still need to perform numerical convergence study

• Future work will focus on two kinetic species: both electrons and ions