An Overview of Fundamental R&D Problems in Space Propulsion (and Related Environment)

4rd Divisional (RQR) 6.1 Review
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• The problems

1. What are we trying to solve? (challenge)
2. Why? (relevance)
3. How do we solve them? (approach)
4. How well do we solve them? (status)
5. How else do we solve them? (alternatives)
6. What did we not solve? (future work)
7. Summary
1: Problems to solve

• Problems being solved (now):
  – Complex (multiscale) plasma chemistry:
    • Collisional-Radiative: 1F, multi-F, non-Maxwellian
  – Multiscale dynamics:
    • $m_e/M << 1$, $\omega_{ce}\Delta t >> 1$, $c\Delta t >> v$, $\omega_{pe}\Delta t >>> 1$
  – Multiscale density:
    • Impact on: statistics, EOS, models….

• Problems remaining:
  – Radiation transport
  – Instabilities, Turbulence
  – Physical models (XS, rates, EOS..)

Problems defined by complexity of interactions. Found elsewhere, but dealing with unique aspects.
2: Why these problems?

• Core applications:
  – Plasma thruster M&S: HET and FRC
  – Plasma spacecraft environment: plumes, SSA, contamination, damage
  – Plasma diagnostics: LIBS, absorption tomography…

Q: How well are we solving these core issues?

• Core Extension:
  – Laser plasma interactions (LPI): hyper-spectral diagnostics, weapon effectiveness, propagation…
  – Space weather?: solar and geomagnetic flows

Q: How are the prospects for contributing to these problems?
2: Core Applications

- **HET**
  - Performance
  - Instabilities
  - Contamination/damage
  - Signature (SSA)

- **FRC**
  - Performance
  - Instabilities
  - Diagnostics
  - Design
2: Core Extension

- LPI
  - RQ experiment (target = liquid)
  - Interaction with density profile
  - Conditions favorable to RT instability
  - Ponderomotive forces important!

- Space weather?
  - Similar problems to Core: multiscale dynamics and chemistry, instabilities, magnetized plasma

Synergy between Core + Extension. Room for expansion if resources available.
3: Scope of R&D

1) Multiscale Collisional-Radiative Kinetics ("chemistry")
   - Hierarchy of complexity:
     • Single-fluid / MHD
     • Multi-fluid / MHD / Maxwell
     • Non-Maxwellian (discrete & MC)

2) Multiscale Transport ("dynamics")
   - LHS of FP/Boltzmann = streaming operator
   - Different directions: PIC, Vlasov, Hybrid
   - Anisotropic effects (magnetized)

3) Multiscale Couplings (additional physics)
   - How to integrate sub-scale physics: MD → MC → Cont.
   - Fluid/Solid coupling (LPI, HET), non-ideal properties
   - Electromagnetic phenomena

Focusing on most important issues (1,2) = basis of M&S capability.
3: Multiscale CR

• Past:
  – 1D and 2D coupled 1F-CR
  – Complexity Reduction
  – Non-Maxwellian discrete model

• Present
  – Multi-Fluid CR model development
  – Non-Maxwellian stochastic model

• Future
  – Multi-species & dynamic reduction
  – RHS to Vlasov
  – PIC integration
  – Radiation transport
3: Multiscale Transport

• **Past**
  - PIC development:
    • GPU-implemented PIC
    • Implicit PIC (Lapenta, Brackbill)
  - Time-parallel acceleration

• **Present**
  - Vlasov: basics being implemented/tested
  - PIC: complexity reduction (merging)
  - MHD: introduction of DG/FE

• **Future**
  - CR coupling: CR-PIC, CR-Vlasov-FP
  - Hybrid: Vlasov-Fluid, PIC-Vlasov-Fluid, $\delta f$
3: Multiscale Physics

• **Past:**
  – XS databases for Ar, Xe, Kr
  – CR complexity reduction

• **Present:**
  – Working with collaborators to extend CR to molecular plasma
  – Some introduction to MD-based sputtering

• **Future:**
  – Micro-physics averaging:
    • MD sputtering database, SEE, CR cross-sections / rates…
    • Sub-grid turbulence (MHD)
  – Non-ideal properties:
    • Fermi statistics (CR), Debye-Hückel, Thomas-Fermi…
4: Status

• Discussed in more detail by accompanying talks…
  
  — Col-Rad:
    • Fluid: 1F done, MF in progress – needs more data
    • Discrete: found instability – needs limiter / FP term?
    • MC: particle merging OK – see also UCLA work (Caflisch-Yan)
    • Molecular CR: collaboration
    • RT: planning stage…
  
  — Transport:
    • CFD: 1F, MF implemented – need GPU optimization
    • PIC: implicit scheme not integrated yet – needs more thought
    • TP acceleration: ambiguous results – switch to other approaches
    • Vlasov: basic schemes tested, working – needs FP, GPU accel., improved accuracy, robustness to magnetized conditions…
    • Hybrid: still mostly on drawing board…
  
  — Coupling:
    • Need consistent XS-rates database (diagnostics, signature…)
    • Need MD-based models integrated (“averaging” operators + UQ ?)
    • Need extension of physical regimes (e.g. Fermi-CR, EOS)

Last item less urgent (→ 6.2). Some resource limitations.
5: Alternatives

- **Chemistry:**
  - Similar work in EU:
    - Variable quality / focus…
    - Leverage? Possible in certain areas → integration effort
  - DOE work: higher energy (useful for LPI) - TBD

- **Transport:**
  - Implicit PIC at LANL
    - But still need integration effort
  - Lots of Vlasov work (US, EU universities)
    - Mostly fusion (tokamak) related…
    - Possible collaboration with U-Michigan
  - Recent Hybrid Vlasov-Fluid (Germany)
    - We are on the right track….

- **Coupling:**
  - Looking for leverage in most areas
  - Focus on integration (→ 6.2)

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*Be aware! If integration effort ≈ development effort, → no leverage.*
*Still evaluating best options.*
6: Remaining Work

• Lots to do, besides completing started efforts:
  – Need to couple/integrate CR and MHD solvers at ALL levels
    • Multi-D, Multi-Species, Radiation transport
    • PIC – Vlasov – MultiF – MHD(1F)
  – Need to improve accuracy/efficiency of some solvers
    • Ensure conservations (variational, projection integrators?)
    • Magnetized transport stiffness (PIC and MHD)
  – Need to increase effort on modeling instabilities
    • HET/magnetron: drift-waves, ionization…
    • FRC: Rayleigh-Taylor (RT), Kelvin-Helmholtz

6: Remaining Work – Ex: instabilities

• **Relevance/Specialization:**
  – FRC propulsion:
    • Current sheet development (shear at FRC interface)
    • Stability and mass capture efficiency
  – Important Characteristics & Differences:
    • Collisionality with neutrals (partially ionized)
    • Tangential B-field (orientation-dependent)
    • Also found in laser fusion and solar prominences
    • Potentially relevant to upper-atmospheric physics
      Mahalov, Phys. Scr. 89 (2014)
6: Remaining Work – Ex: instabilities

- RT Example: Crab Nebula

- Growth of filamentary structures
- Generation/concentration of EM fields
- Mixing of elements/chemistry

6: Remaining Work – Ex: instabilities

• Previous FRC modeling
  – Implicit PIC
  – \( m_e \times 10 \)
  – Theta-Pinch configuration
  – Flute (RT) instability

\[ g \propto -\nabla P \]

\[ V_D = \frac{F \times B}{eB^2} = \frac{M g \times B}{eB^2} \]

\[ V_H = \frac{E \times B}{B^2} \]

Ion drift → charge separation → Hall drift

Unstable!

– Is it real? (given enough time)
  • \( m_e/M \) still small enough
  • Assumed fully ionized…
  • Assumed no initial shear…
6: Remaining Work – Ex: instabilities

- KH example: instability
  - Relevant to current sheet stability?
  - Suppressed/Enhanced by B field
  - Similar effect was previously studied (RT)

*Fundamental* studies compatible with development & application of M&S capability for Core + Extension projects.
7: Summary

• Several projects at the forefront of modern physics and mathematical methods
• Supports overall R&D objectives in plasma propulsion
• Progress made in various areas:
  – Moving towards *Big-Challenge* project in CR
  – Various (promising) options for transport actively pursued
  – Need more algorithm work (accuracy/stiffness)
  – Need additional physics: databases, properties and models (→ 6.2)
• Fundamental work, can be applied to other areas
  – rev: work in other areas can be leveraged)
• Challenging and *exciting* projects….
• Stretched resources…
6: Remaining Work

• Multiple: drift-wave, Rayleigh-Taylor (RT) and Kelvin-Helmholtz (KH)
  – RT: Driven by forces normal to interface (gravity, pressure)
  – KH: Driven by forces tangential to interface (shear)
  – Prelude to turbulence
  – Critically important for:
    • Astrophysics (Supernovae, Nebulae, Solar prominences)
    • Inertial Fusion (mixing)
• **FRC modeling**
  - Implicit PIC
  - $m_e \times 100$
  - Theta-Pinch configuration
  - Flute (RT) instability
  - Is it real?

\[ V_{VD} = F \times B - \frac{M g \times B}{e B^2} \]

\[ \nabla \nabla P \]

\[ V_{VH} = \frac{E \times B}{B^2} \]

Ion drift → charge separation → Hall drift

**Unstable!**
• **FRC modeling**
  - Implicit PIC
  - $m_e \times 10$
  - Theta-Pinch configuration
  - Flute (RT) instability
  - Is it real?

\[ B^2 = V_D = F \times B \times \frac{M g \times B}{e B^2} \quad V_H = \frac{E \times B}{B^2} \]

Ion drift $\rightarrow$ charge separation $\rightarrow$ Hall drift

**stable!**
• **FRC modeling**
  - Implicit PIC
  - \( m_e \times 100 \)
  - Theta-Pinch configuration
  - Flute (RT) instability
  - Is it real?

\[
\begin{align*}
V_D &= \frac{F \times B}{eB^2} = \frac{M g \times B}{e B^2} \\
V_H &= \frac{E \times B}{B^2}
\end{align*}
\]

Ion drift → charge separation → Hall drift

Unstable!
• **FRC modeling**

  - Wait! Remember that $m_e$ is not physical

  $$V_D = \frac{M \mathbf{g} \times \mathbf{B}}{e B^2} \propto -\frac{\nabla P}{eNB} \propto -\frac{1}{L_V} \frac{kT}{eB}$$

  - $T$ unchanged: $V_D$ does not depend on $M \rightarrow$ OK

  - Other drift? Field curvature….

  $$V_D = \frac{M}{e} \left( \frac{v_1^2}{2} + v_\parallel^2 \right) \frac{R_c \times B}{R_c^2 B^2} \propto \frac{P}{eNR_cB} \propto \frac{1}{R_c} \frac{kT}{eB} \rightarrow$ OK
Nature of Multiscale Problems

• Traditional approach: projection operator

  – Scale separation: \( y = y_s + y_f \)

    • when \( \varepsilon \to 0 \), solve \( \frac{dy_f}{dx} = \frac{1}{\varepsilon} f_1(y_s, y_f, x) \)

    • Use "relaxed" solution for \( \frac{dy_s}{dx} = f_0(y_s, y_f^*, x) \)

    • Works best if \( M_s \cap M_f = \emptyset \)

      – Implies eigen-decomposition ($$)

    • If dynamics become constrained on \( M_s \)

      Slow manifold \( \equiv \) Invariant manifold
Nature of Multiscale Problems

- Works if slow manifold is "attractive"
  - Negative real eigenvalues
- Could work if \( \exists \) basin of attraction
  - Allows for some imaginary eigenvalues (bounded)

- Ex: electron trajectories in PIC
  - Need to model plasma oscillations? In most cases, no.
Nature of Multiscale Problems

• Complications:
  – Positive eigenvalues:
    • invariant manifold = repulsive fixed point (saddle)
    • Ex: instability, inverse cascade…
  – Chaotic regime:
    • no invariant manifold (not of interest)
  – Stochastic fine scales:
    • Need statistical model
    • Ex: e- trajectories + collisions
  – Non-separation of scales:

\[
\frac{dy}{dx} = f_0(y, x) + \frac{1}{\varepsilon_1} f_1(y, x) + \frac{1}{\varepsilon_2} f_2(y, x) + \ldots
\]
Nature of Multiscale Problems

• Complications:
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\[ \frac{dy}{dx} = f_0(y, x) + \frac{1}{\varepsilon_1} f_1(y, x) + \frac{1}{\varepsilon_2} f_2(y, x) + \ldots \]

Real structure can be very complex…