STABILIZED FINITE ELEMENT MODELING OF PLASMA FLOW INSTABILITIES

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Outline

1. Introduction & Background (why it is important)
2. Mathematical Model (what we know)
3. Numerical Model (how to deal with it - 1)
4. Solution Approach (how to deal with it - 2)
5. Preliminary Results (where we are)
6. Conclusions & Further Work (what’s next)
SciDAC needs methods for the solution of general multiphysics-multiscale problems

- Methods that rely as little as possible on deep analysis of equations

**Promising**: Stabilized and Multiscale Methods
**Definition of Plasma**

**Plasmas:**
- Partially or fully ionized gases
- Any gas mixture with charged species, i.e. $\text{Ar} + M \rightarrow \text{Ar}^+ + e^- + M$
- +99% of observable mass in the universe
- 4$^{\text{th}}$ state of matter: *solid → liquid → gas → plasma*

- Typically, span over a wide range of scales …

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[Diagram showing the transition from solid to gas to plasma with temperature scale from cold to hot]
Plasmas: From natural phenomena ... to tech. applications

Motivation of this Research

• Thermal plasmas widely used for materials processing

• Applications show inconsistent results due to instabilities
  ➢ Characteristic process time in same order as instability
  ➢ Example: plasma spray coating

- Need better understanding of plasma dynamics -

Goal of this research: Develop a computational model capable of describing flow in plasma torches and predicting effects of design and operating parameter changes
Arc and Jet Dynamics

- arc length $\propto$ voltage drop
- imbalance Drag-Magnetic forces
- arc movement $\rightarrow$ jet forcing
- enhanced cold flow entrainment
Reattachment Process

1. attachment movement

2. new attachment appears

3. new attachment remains

experiments, simplified geometry

**Stability**

- Commonly related to potential energy curves:

  - stable
  - unstable
  - neutrally stable
  - metastable

- **Lyapunov**: if all points that start near $x$ stay near $x$ forever
  $\rightarrow x$ is Lyapunov stable

- **Are arc dynamics due to instability?**

```
+ stable
unstable
```

![Graph showing voltage (V) over time (ms)](image)
**Plasma Flow Instabilities**

- **Fluid:** shear instability $\rightarrow$ uncond. unstable $T_1/T_2 > 1.52$ (> 10 in plasma!)

- **Magnetic:** kink and sausage instabilities (but too low $B$?)

- **Thermal:** cold flow interaction

- **Electrical:** not considered here (RLC characteristic of system)
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A Hierarchy of Plasma Models

- **Particle Models**
  - Molecular Dynamics (MD)
  - Monte Carlo (DSMC)
  - Particle-in-Cell (PIC)
  - ...

  - Particle or Fluid model best depending on problem
  - A single model may not be valid in the whole domain of interest

- **Fluid Models**
  - Boltzmann (time + 6D phase space)
  - Multi-fluid \((\rho_s, u_s, T_s\) for each species \(s\))
  - Chemical & thermal non-equilibrium (multiple species, temperatures)
  - Chemical & thermal equilibrium
  - Equilibrium & inviscid

  \[
  \frac{\partial f_s}{\partial t} + \bar{u} \cdot \nabla_x f + \bar{a} \cdot \nabla_u f = f_s^c
  \]

  simpler, less accurate

in this research
Mathematical Approach: LTE Model

- **Fluid** (conservation eqns.) + **Electromagnetic** (Maxwell’s eqns.) + Thermodynamic & Transport Properties
- System of Transient-Advective-Diffusive-Reactive eqns. for: \( p, \bar{u}, T, \phi, \bar{A} \)

<table>
<thead>
<tr>
<th>transient</th>
<th>advection</th>
<th>diffusion</th>
<th>reaction</th>
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<tbody>
<tr>
<td>( \frac{\partial p}{\partial t} )</td>
<td>( \nabla \cdot \rho \bar{u} )</td>
<td>( \rho \bar{u} \cdot \nabla \bar{u} - \nabla p )</td>
<td>( - \nabla \cdot \mu \left( \nabla \bar{u} + \nabla \bar{u}^T - \frac{2}{3} \nabla \cdot \bar{u} \bar{\delta} \right) )</td>
</tr>
<tr>
<td>( \rho \frac{\partial \bar{u}}{\partial t} )</td>
<td>( \rho \bar{u} \cdot \nabla \bar{u} - \nabla p )</td>
<td>( \nabla \cdot (\kappa \nabla T) - \frac{k_B}{e} \bar{J}_q \cdot \nabla T )</td>
<td>( - \left( \bar{J}_q \cdot \bar{E} - Q_r - \frac{\partial \ln \rho}{\partial \ln T} - \frac{Dp}{Dt} \right) )</td>
</tr>
<tr>
<td>( \rho C_p \frac{\partial T}{\partial t} )</td>
<td>( \rho C_p \bar{u} \cdot \nabla T )</td>
<td>( \nabla \cdot (\kappa \nabla T) - \frac{k_B}{e} \bar{J}_q \cdot \nabla T )</td>
<td>( - \left( \bar{J}_q \cdot \bar{E} - Q_r - \frac{\partial \ln \rho}{\partial \ln T} - \frac{Dp}{Dt} \right) )</td>
</tr>
<tr>
<td>( \mu_0 \sigma \frac{\partial \bar{A}}{\partial t} )</td>
<td>( \mu_0 \sigma \left( \bar{u} \times \nabla \times \bar{A} - \nabla \phi \right) )</td>
<td>( \nabla^2 \bar{A} )</td>
<td>( - \nabla \cdot \sigma \left( \nabla \phi - \bar{u} \times \nabla \times \bar{A} \right) )</td>
</tr>
</tbody>
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Additional: \( \rho = \frac{p}{R_g T}, \quad \bar{B} = \nabla \times \bar{A}, \quad \bar{E} = -\nabla \phi - \frac{\partial \bar{A}}{\partial t}, \quad \bar{J}_q = \sigma (\bar{E} + \bar{u} \times \bar{B}), \quad \bar{E}' = \bar{E} + \bar{u} \times \bar{B} \)
Mathematical Approach: Non-Equilibrium Model

- Thermal and chemical non-equilibrium
- System of transient advection-diffusion-reaction equations (TADR):

\[
\begin{align*}
\text{transient} & + \quad \text{advection} & + \quad \text{diffusion} & - \quad \text{reaction} & = 0 \\
1. \text{Mass cons.} \quad & \frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{u} \rho) & & = 0 \\
2. \text{Species cons.} \quad & \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\vec{u} \rho_s) + \nabla \cdot \vec{J}_s & - \quad \rho_s & = 0 \\
3. \text{Momentum} \quad & \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\vec{u} \rho \vec{u}) + \nabla \cdot \vec{P} & - \quad \vec{J}_q \times \vec{B} & = 0 \\
4. \text{En. Elect.} \quad & \frac{\partial \rho_e e_e}{\partial t} + \nabla \cdot (\vec{u} \rho_e e_e) + \nabla \cdot \vec{q}' & - \quad \left( \vec{J}_q \cdot \vec{E}' - \dot{Q}_{eh} \vec{Q}_{eh,e} - \dot{Q}_r - P \nabla \cdot \vec{u} \right) & = 0 \\
5. \text{En. Heavy} \quad & \frac{\partial \rho_h e_h}{\partial t} + \nabla \cdot (\vec{u} \rho_h e_h) + \nabla \cdot \vec{q}_h & - \quad \left( \dot{Q}_{eh} - P \nabla \cdot \vec{u} \right) & = 0 \\
6. \text{Ampere's law} \quad & \nabla \times \vec{B} & - \quad \mu_0 \vec{J}_q & = 0 \\
7. \text{Current cons.} \quad & \nabla \cdot \vec{J}_q & = 0 
\end{align*}
\]
Thermodynamic & Transport Properties

- Strongly non-linear properties:
  - function of composition (chemical non-equil.)
  - function of temperatures (thermal non-equil.)

>>> properties can vary by orders of magnitude! <<<
Dealing with Non-Linear Properties

- **Example:** Poisson eqn. (current conservation)
  \[ \nabla \cdot (\sigma \nabla \phi) = 0 \quad \& \quad \sigma(T) \]

  >> Galerkin doesn’t work where
  \( \nabla T \) large (oscillations)

- **1st approach:** advection-diffusion eqn.
  - Treat \( \sigma \) as \( \sigma(X) \):
    \[ \nabla \sigma \cdot \nabla \phi + \sigma \nabla^2 \phi = 0 \]
  - Needs adaptive refinement:
    \[ h < \frac{\sigma}{|\nabla \sigma|} \quad - h \text{ extremely small} \]
  - Or stabilization (i.e. SUPG)
Dealing with Non-linear Properties (cont.)

2\textsuperscript{nd} approach: two-var. advection-diffusion eqn.

- Treat $\sigma$ as $\sigma(T)$:
  \[
  \left( \frac{\partial \sigma}{\partial T} \right) \nabla T \cdot \nabla \phi + \sigma \nabla^2 \phi = 0
  \]
- Need adaptive refinement or stabilization, but how?
- Recall: $\nabla T$ can be very large

3\textsuperscript{rd} approach: multi-var. advection-diffusion eqn.

- $\sigma$ is actually $\sigma(T, \rho_e, \ldots)$:
  \[
  \left( \frac{\partial \sigma}{\partial T} \right) \nabla T + \left( \frac{\partial \sigma}{\partial \rho_e} \right) \nabla \rho_e + \ldots \cdot \nabla \phi + \sigma \nabla^2 \phi = 0
  \]
- Adaptive refinement or stabilization??

Now, what if instead of Poisson:

\[
\nabla \cdot (\sigma \nabla \phi) + \nabla \cdot \sigma \left( \frac{\partial \vec{A}}{\partial t} - \vec{u} \times \nabla \times \vec{A} \right) = 0
\]

Adding more physics makes things harder!
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The TADR System

- System of **TADR** equations:

\[
A_0 \frac{\partial Y}{\partial t} + (A \cdot \nabla)Y - \nabla \cdot (K \nabla Y) - (S_1 Y + S_0) = 0
\]

- This is \sim \text{ arbitrary. In a code, we really need:}

\[
A_0, A, K, S_1, S_0 \quad \text{functions of} \quad t, X, Y, \nabla Y, \dot{Y},...
\]

- Many, many fluid flow problems can be treated as **TADR**, including:
  - Multi-fluid models \quad (3D)
  - Relativistic fluids \quad (4D)
  - Boltzmann equations \quad (6D)

- Yet, very few work on general **TADR** systems …
Finite Element Method

TADR equations:

\[
\frac{A_0}{\partial t} \partial Y(t) + (A \cdot \nabla) Y - \nabla \cdot (K \nabla Y) - (S_1 Y + S_0) = \nabla Y - S_0 = R(Y) = 0
\]

- **Galerkin FEM:**
  \[W = \text{weight function} = \text{basis function} = N(X)\]
  \[\Omega \quad \text{Spatial domain}\]
  \[\Gamma_1 \quad \text{Dirichlet boundary:} \quad Y = Y_{\text{fix}}\]
  \[\Gamma_2 \quad \text{Robin boundary:} \quad K \partial_n Y + q_0 + q_1 Y = 0\]

- **Integration by parts:**
  \[\int_{\Omega} N^T (A_0 \partial Y/\partial t + (A \cdot \nabla) Y - (S_1 Y + S_0)) + \int_{\Omega} \nabla N^T (K \nabla Y) + \int_{\Gamma_2} N^T (q_0 + q_1 Y) = 0\]

**Problem:** doesn't work incompatible and/or unresolved discretizations
  \[\rightarrow \text{doesn't work for multiphysics-multiscale problems}\]
Typical example:

“different characteristic sizes needed to describe different parts of the process”
A Canonical Multiscale Problem

Supersonic flow over a sphere – different length scales

mean flow \( l \sim O(L) \)

flow direction

boundary layer \( l \sim O(L/Re)^{1/2} \)

shocks \( l \sim O(\lambda) \)

turbulent wake \( l \sim O(L \text{ to } L/Re) \)

Tremendously difficult to model with today’s methods!

Recall:
\[
Re = \frac{\rho UL}{\mu}
\]

* M. Van Dyke, An Album of Fluid Motion, 1982
Variational Multiscale Methods

- Scale decomposition: $\mathbf{Y} = \mathbf{\bar{Y}} + \mathbf{Y}'$
- Related to stabilized methods (i.e. SUPG, GLS)

$$\text{total} = \int_{\Omega} \mathbf{W} \mathbf{R}(\mathbf{Y}) d\Omega + \int_{\Omega'} \mathbf{P}(\mathbf{W}) \mathbf{\tau R}(\mathbf{Y}) d\Omega' = 0$$

“A Framework for the Solution of General Multiphysics-Multiscale Problems”

$\gg$ extra term $\to 0$ as mesh is refined (approach DNS)

$\gg$ ~only alternative for modeling, i.e., turbulent reactive electromagnetic flows
Stabilized & Multiscale Finite Element Methods

- Generalization:
  \[ P = \mathcal{L}_{\text{adv}} \text{SUPG} \]
  \[ P = \mathcal{L} \text{ GLS} \]
  \[ P = -\mathcal{L}^* \text{ VM} \rightarrow \text{ASGS} \]

- Problem becomes:

\[
\int_{\Omega} N^T \left( A_0 \frac{\partial Y}{\partial t} + (A \cdot \nabla)Y - S_1 Y - S_0 \right) + \int_{\Omega} \nabla N^T (K \nabla Y) + \int_{\Gamma_2} N^T (q_0 + q_1 Y) \]

Galerkin

\[
\int_{\Omega'} P(N)^T \boldsymbol{\tau}_{SGS} \mathcal{R}(Y) + \int_{\Omega'} \nabla N^T (K_{DC} \nabla Y) = 0
\]

sub-grid scale term

\[ \text{discontinuity capturing} \]

>> Consistency: residual based, extra terms → 0 as mesh is refined

>> **Still need to define:** \[ \boldsymbol{\tau}_{SGS} \& \ K_{DC} \]
Intrinsic Time Scales Matrix, $\tau^{SGS}$

- **Formally:** $\tau = \frac{1}{\text{meas}(\Omega_e)} \int \int g'(x,y) dx dy$ (Hughes et al) How to find $g'$?

  \[ 1D \text{ adv-diff: } \tau = \frac{h}{|a|} \xi(Pe), \quad Pe = \frac{|a|h}{k} = \text{adv. diff.} \]

- **Empirically:** ($\sim$ generalizations of 1D)

  \[ \tau \approx h |A|^{-1} \xi(Pe, Co, Da, ...) \quad Pe = \frac{\text{adv. diff.}}{\text{diff.}}, \quad Co = \frac{\text{adv. trans.}}{\text{trans.}}, \quad Da = \frac{\text{adv. react.}}{\text{react.}} \]

  i.e. $\tau \approx \left( c_1 \left| \frac{A_0}{\Delta t} \right|^p + c_2 \left| \frac{A}{h} \right|^p + c_3 \left| \frac{K}{h^2} \right|^p + c_4 \left| \frac{S_1}{1} \right|^p \right)^{-\frac{1}{p}}$ (Shakib, Hauke, Tezduyar, Codina)

- **In this research:** (LTE) $\tau = \text{diag}(\tau_c, \tau_m, \tau_m, \tau_m, \tau_e, 0, 0, 0, 0)$
Discontinuity Capturing Diffusivity Matrix, $K_{DC}$

- Needed because formulation does not preserve monotonicity (or because $\tau$ is not well approximated?)

Hughes & Mallet, Hughes & Shakib, Tezduyar, …

$$K_{DC} = \left\{ v_{DC} A_0 g^{ij} \right\} \quad \text{with} \quad v_{DC} = 2 \frac{\mathcal{R}(Y) \cdot \tau \mathcal{R}(Y)}{g^{ij} Y_{,i} \cdot Y_{,j}} \quad \text{(scalar)}$$

$>>$ acts // to $\nabla Y$, negligible if smooth solution ($\mathcal{R}(Y) \sim 0$)

$>>$ method non-linear even for linear problems

$>>$ **Problem** (?) : $K_{DC}$ adds the same dissipation to all the variables

- **In this research:** (similar to Codina’s; only to variables that need it)

$$K_{DC}(y) = \frac{h_y}{2|\nabla y|} |\mathcal{R}(y)| \chi_y$$
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Discrete System

- **Newton Method**: \( \text{Res}(Y) \to 0 \implies \text{Jac} \Delta Y \approx -\text{Res}, \quad \text{Jac} = \partial \text{Res}/\partial Y \)

- **Residual vector**:

\[
\text{Res} = A_e \text{Res}_e
\]

\[
\text{Res}_e = \int_{\Omega_e} N^T \left( A_0 \frac{\partial Y}{\partial t} + (A \cdot \nabla) Y - S_1 Y - S_0 \right) + \int_{\Omega_e} \nabla N^T (K \nabla Y) + \int_{\Gamma_{2e}} N^T (q_0 + q_1 Y) + \int_{\Omega_e} \mathcal{P}(N)^T \boldsymbol{\tau}_{SGS} \mathcal{R}(Y) + \int_{\Omega_e} \nabla N^T (K_{DC} \nabla Y)
\]

- **Jacobian matrix**: (approx., frozen coeff.)

\[
\text{Jac} = A_e \text{Jac}_e
\]

\[
\text{Jac}_e = \int_{\Omega_e} N^T ((A \cdot \nabla) - S_1) N + \int_{\Omega_e} \nabla N^T (K \nabla N) + \int_{\Gamma_{2e}} N^T (q_1 N) + \int_{\Omega_e} \mathcal{P}(N)^T \boldsymbol{\tau}_{SGS} \mathcal{R}(N) + \int_{\Omega_e} \nabla N^T (K_{DC} \nabla N)
\]
Solver Layout

Need to solve: \( \text{Res}(t, X, Y, \dot{Y}) \rightarrow 0 \)

Loop: Time stepping
- Second order implicit predictor-multicorrector

Loop: Solution non-linear system
- Globalized Newton-Krylov method

\[ \left\| \text{Res} + \text{Jac}\Delta Y^{k+1} \right\| \leq \eta \left\| \text{Res} \right\| \]
\[ Y^{k+1} = Y^k + \lambda \Delta Y^{k+1} \]

Loop: Solution linear system
- Preconditioned Generalized Minimal Residual (GMRES)

\[
\begin{align*}
Ax &= b \\
(P^{-1}A)x &= (P^{-1}b)
\end{align*}
\]
Time Stepping

- Solution of $\text{Res}(Y, \dot{Y}) = 0$ by 2nd order, implicit, predictor multi-corrector, with control of high frequency amplification

\[
\frac{Y_{n+1} - Y_n}{\Delta t} = (1 - \alpha_f) \dot{Y}_n + \alpha_f \dot{Y}_{n+1}
\]

\[
Y_{n+\alpha_f} = (1 - \alpha_f) Y_n + \alpha_f Y_{n+1}
\]

\[
\dot{Y}_{n+\alpha_m} = (1 - \alpha_m) \dot{Y}_n + \alpha_m \dot{Y}_{n+1}
\]

\[\text{Res}(Y_{n+\alpha_f}, \dot{Y}_{n+\alpha_m}) = 0\]

- For higher order use BD methods (i.e. Sundials’ IDA solver)
- $\alpha$-method or BD only need: Res and Jac for a given $Y_n, \dot{Y}_n, \zeta = \frac{\partial Y_n}{\partial Y_n}$

- Need solution of non-linear system at each time step
Solution of Non-Linear System

• **Needed:** minimum function evaluations (expensive for complex physics → matrix–free, pseudo-trans. not very attractive)


\[
\left\| \text{Res} + \text{Jac}\Delta Y^{k+1} \right\| \leq \eta \|\text{Res}\|
\]

\[
Y^{k+1} = Y^k + \lambda \Delta Y^{k+1}
\]

>> Forcing term \( \eta \): Eisenstat-Walker

>> Backtracking: Armijo condition

>> Line search \( \lambda \): Parabolic - three point interpolation

* Backtracking essential when \( \Delta t \) still large
  (too large change in solution)
Solution of Linear System

• Generalized Minimal Residual (GMRES) with restarts + …

• Scaling: (unavoidable, unless dimensionless variables are used)
  \[ D^{-1}Ax = D^{-1}b \quad \rightarrow \quad \tilde{A}x = \tilde{b}, \quad D = \text{diag}(A) \]

• Pre-preconditioning: (something to do to \( A \) and \( b \) before linear solve)
  \[ P_0^{-1}\tilde{A}x = P_0^{-1}\tilde{b} \quad \rightarrow \quad \tilde{A}x = \tilde{b}, \quad P_0 = \text{block \_ \ diag}(\tilde{A}) \quad \text{(EBE)} \]

• Preconditioning: (as usual)
  \[ P^{-1}\tilde{A}x = P^{-1}\tilde{b} \quad \rightarrow \quad \tilde{A}x = \tilde{b}, \quad P = \ldots \]

<table>
<thead>
<tr>
<th></th>
<th>ILU(0)</th>
<th>ILU(tol)</th>
<th>Add. Schwz.</th>
<th>EBE-GS</th>
<th>BlkDiag</th>
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<tr>
<td>Scaling</td>
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<td>PreCond</td>
<td>X</td>
<td>X</td>
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</tr>
</tbody>
</table>

best (least expensive)
Verification & Validation

- Van Der Pol: \[ y'' + \nu(1 - y^2)y + y = 0; \text{ as } \nu \uparrow \Rightarrow \text{stiffer problem} \]

\[ \alpha \text{-method vs. Matlab's ODE 115s (variable order BD)} \]

- Driven cavity flow:
  - tested different Re
  - unsteady for Re > ~5000?

* same solver, only change: \( A_0, A, K, S_1, S_0, \tau_{SGS}, K_{DC} \)
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   Conditions: Ar-He (75-25), 60 slpm, 800 A, straight injection

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Computational Domain $\Omega$

- 3 cases: 
  a) torch coarse 380k dof
  b) torch fine 620k dof
  c) torch + jet 850k dof
- hexahedral trilinear elements
- d.o.f. per node: 9 for LTE model (+11 for Non-Equil.)
Solution Parameters/Statistics

Time Advancement: \( \Delta t \sim 0.1 - 1.0 \) μs
\( nt \sim 500 - 1000 \) (each reattachment period \( \sim 100 \) μs)

Non-linear Solver: \( \sim 5 \) Inexact Newton ites. /\( \Delta t \)
\( \eta_0 = 1.0^{-2}, \eta_{\text{max}} = 1.0^{-3} \)
Backtracking needed @ beginning of reattachment
Stop: \( |\text{Res}|/|\text{Res}_0| \leq 0.1 \) & \( |\Delta Y|/|Y| \leq 1.0^{-3} \)

Linear Solver: Krylov space 30 x 5 restarts = 150 ites. /In. Newton
Scaling + Blck Diag. Pre-Preconditioner + No Preconditioner

\( nt: 474, t: 2.27e-04 \)
\( > \) Reattachment process begins
ite: 1, out/in: 2/ 4, fevals: 4, red: 2, flag: 0, lam: 0.25, eta: 1.00e-02, errY: 3.62e-02, errR: 1.00e+00
ite: 2, out/in: 1/14, fevals: 1, red: 0, flag: 0, lam: 1.00, eta: 5.62e-03, errY: 7.85e-01
ite: 3, out/in: 2/12, fevals: 1, red: 0, flag: 0, lam: 1.00, eta: 3.16e-03, errY: 2.34e-01
ite: 4, out/in: 2/19, fevals: 1, red: 0, flag: 0, lam: 1.00, eta: 1.78e-03, errY: 1.40e-01
ite: 5, out/in: 3/26, fevals: 1, red: 0, flag: 0, lam: 1.00, eta: 1.00e-03, errY: 9.76e-02
errSS: 2.06e-02, dtnew = 3.06e-07, SFAC = 1.07
Instantaneous temperature distribution inside the torch

Conditions: Ar-He (75-25), 800 A, 60 slpm, straight injection
Reattachment Process

- Attachment when arc close enough to anode
- Too long arc, high voltages → Reattachment Model needed
Reattachment Process – with Reattach. Model

- Insert high $\sigma$ column where $|E_r| > E_0$
- Limits arc length, voltage drop ~ mimics physical reattach

new attachment
Arc Dynamics

original attachment

Electric potential over 14000 K isosurface
\[ u_{in} \sim 30 \text{ [m/s]} \]
\[ Mach_{in} \sim 0.01 \]

\[ u_{out} +2500 \text{ [m/s]} \]
\[ Mach_{out} \sim 0.70 \]

➢ from incompressible to compressible
Electric and Magnetic Potentials & Fields

- electric potential
  ~ independent of arc movement

- magnetic potential
  indicates position of arc
Arc and Jet Dynamics

Conditions: Ar-He (75-25), 800 A, 60 slpm, straight injection

- Turbulent jet clearly under-resolved
- Excessive damping
Arc Movement as Jet Forcing

simulation

experiment
Time Evolution of Arc Characteristics

*Conditions: Ar-He (75-25), 800 A, 60 slpm, swirl 45°*

- Simulation
  
  ![Simulation Graph](image)

- Experiment
  
  ![Experiment Graph](image)

- Main frequency agrees BUT amplitude doesn't
- Overall adequate description of arc dynamics
Non-LTE Model - Preliminary Results (2D)

- Axisymmetric, chemical equilibrium, two temperatures

- Thicker cold boundary layer

- Highest non-equilibrium

- Artificially high $\sigma$ in front of anode not needed
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Temperature Distribution [kK] and Velocity Vectors
Conclusions & Further Work

• Developed: $n$-dimensional, transient, fully coupled, Stabilized/Multiscale-FEM solver for modeling TADR eqns.

• Results of LTE modeling of plasma flow:
  ▪ some aspects of arc dynamics revealed
  ▪ reasonable agreement with experiments

• Thermal and chemical non-equilibrium model under development (less assumptions, more physics)

• Code parallelization: C + MPI + PETSc
  (domain decomposition + NLS solver + Add. Schwarz)

• Study of plasma flow instability: eigenvalue analysis, forcing (need accurate $\text{Jac}$, effect of stabilization on stability?)
Stability Diagram

- **Input**: Operating parameters  
  **Output**: Main frequency
- Simulations ~ primary branch → continuation algorithm needed

\[ St = \frac{fL^3}{Q} \]

Steady, takeover, restrike

\[ Nh = \left( \frac{\rho_0 h_0 \sigma_0}{\text{fluid}} \right) \left( \frac{L}{\text{geometry}} \right) \left( \frac{Q}{I^2} \right) \approx \frac{\text{flow power}}{\text{electric power}} \]

- Key for the design/control of plasma systems
Plasma – Surface Interaction

- Continuum approximation breaks down near surface (too steep gradients, too small distance)

- Hybrid continuum-discrete model needed:
  Continuum: Stabilized/VMS FEM 
  Discrete: Molecular Dynamics

Loosely coupled approach: through Boundary Conditions
We Need a “Universal Solver” for TADR Systems

Solve systems in conservative and/or quasi-linear form:

\[
\frac{\partial U}{\partial t} + \nabla \cdot F - S = 0
\]

\[
A_0 \frac{\partial Y}{\partial t} + (A \cdot \nabla)Y - \nabla \cdot (K\nabla Y) - (S_1 Y + S_0) = 0
\]

- **Variation Multiscale Method**: Define \( A_0, A, K, S_1, S_0 \), etc …
  - + numerical eval. of the SGS term, i.e. mesh sequencing; or …
  - + find \( Y' \) by any other means, i.e. MD … (Heterogeneous Multiscale?)

- **DAE time stepping**: \( \alpha \)-method, variable order BD + adaptive \( \Delta t \)

- **Globalized Newton-Krylov**: GMRES + Line Search

- **Scalable Preconditioners**: Schwarz, AMG

**A U-TADR Solver will boost scientific discovery!**
\[ \nabla \cdot (\sigma \nabla \phi) = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0 \]

\[ \nabla^2 \vec{A} = -\mu_0 \vec{j} \]

\[ \rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p - \nabla \cdot \vec{T} + \vec{j} \times \vec{B} \]

\[ \rho C_p \left( \frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T \right) = \nabla \cdot \vec{q} + \vec{j} \cdot \vec{E}' - U_r + \frac{\kappa_B}{e} \vec{j} \cdot \nabla T \]

\[
\int_{\Omega} W R(Y) d\Omega + \int_{\Omega'} P(W) \tau R(Y) d\Omega' = 0
\]

Thank You
Heterogeneous Variational Multiscale Approach

**HVMS:**

\[
\text{Res}(Y, Y') = \int_{\Omega} W(\mathcal{L}Y - S_0) - \int_{\Omega'} \mathcal{L}^*(W)Y' = 0
\]

**Algorithm:**

1. Estimate \( Y \)
2. Solve for \( Y' \) having \( Y \) as background (i.e. by a particle model, sub-mesh)
3. Project \( Y' \) into \( Y \) space (or higher but consistent)
4. Compute element-level *large* and *small* terms (above)
5. Assemble global residual: \( \text{Res}(Y, Y') \rightarrow \text{Res}(Y) \) (and Jacobian)
6. Update \( Y \) (\( \text{Jac}\Delta Y \approx -\text{Res} \))
7. Go to 1 until convergence
Maxwell’s Equations and $\nabla \cdot B = 0$

- **Maxwell’s equations:**
  1) Ampere’s law: $\nabla \times \vec{B} = \mu_0 \vec{J}_q$
  2) Faraday’s law: $\nabla \times \vec{E} = -\partial \vec{B}/\partial t$
  3) Ohm’s law: $\vec{J}_q = \sigma (\vec{E} + \vec{u} \times \vec{B})$
  4) Gauss’ law: $\nabla \cdot \vec{J}_q = 0$
  5) No magnetic monopoles: $\nabla \cdot \vec{B} = 0$

- **3) in 1) $\rightarrow$ in 2): Magnetic Induction Eqn. (MIE)**

  $$\frac{\partial \vec{B}}{\partial t} - \nabla \times (\vec{u} \times \vec{B}) + \nabla \times (\eta \nabla \times \vec{B}) = 0; \quad \eta = (\mu_0 \sigma)^{-1}$$

- **BUT… $\nabla \cdot \vec{B} = 0$ constraint is missing. To deal with it:**
  - Add extra “divergence” wave $= \text{add source term } \propto \nabla \cdot B$ (Powell et al)
  - Penalty methods (Reddy et al)
  - 4 eqns. $\rightarrow$ 4 unknowns $\Rightarrow$ solve for extra dummy variable (Fortin et al)
  - Others (compatible discretizations, projections, etc.)
Maxwell’s Equations and $\nabla \cdot B = 0$ (cont.)

An alternative: use magnetic and electric potentials…

$$\vec{B} = \nabla \times \vec{A} \quad (\nabla \cdot \vec{B} = 0 \text{ a priori})$$
$$\vec{E} = -\nabla \phi - \partial \vec{A}/\partial t \quad (\text{suggested from } \nabla \cdot \vec{J}_q = 0)$$

Then …

$$\frac{\partial \vec{A}}{\partial t} - \vec{u} \times \nabla \times \vec{A} + \nabla \phi + \eta \nabla \times \nabla \times \vec{A} = 0$$
$$- \nabla \cdot (\sigma \nabla \phi) - \nabla \cdot \sigma \left( \frac{\partial \vec{A}}{\partial t} - \vec{u} \times \nabla \times \vec{A} \right) = 0$$

Why is not the $A$-$\phi$ formulation more popular?

– 4 unknowns (instead of 3 in MIE)
– Cannot be expressed in divergence form
– Harder to specify boundary conditions (needs Gauge condition $\nabla \cdot \vec{A} = 0$)

In this research: no applied $B$ fields $\rightarrow$ BCs not crucial as far as $A$ decays monotonically far from the arc (approx. Biot-Savart law)
Non-Equilibrium Formulation

• Thermodynamic Properties:
  – Mass conservation:  \( n = \sum_{s=0}^{ns} n_s \)
  – Ideal gas:  \( p_s = n_s k_B T_s \)
  – Dalton’s law:  \( p = \sum_{s=0}^{ns} p_s \)
  – Quasineutrality:  \( \sum_{s=0}^{ns} eZ_s n_s = 0 \)
  – Internal energy:  \( e = e_{\text{trans}} + e_{\text{int}} = \frac{3}{2} \frac{k_B}{m} T + \frac{k_B T^2}{m} \left( \frac{\partial \ln Q_{\text{int}}}{\partial T} \right)_V \)
    \( Q_{\text{int}} = \sum g_1 \exp \left( -\frac{\theta_i}{T} \right) \)

• Transport Properties:
  – Chapman-Enskog approximation (Devoto, 1965):  \( f_i = f_i^0 + \xi f_i^1 + \xi^2 f_i^2 + \ldots \approx f_i^0 (1 + \xi \phi_i) \)
    i.e. second order viscosity:
    \[ [\mu] = \frac{-5(2\pi k_B T)^4}{2|\theta|} \begin{vmatrix} \hat{q}_{ij}^{00} & \hat{q}_{ij}^{01} & n_i m_j \hline \hat{q}_{ij}^{10} & \hat{q}_{ij}^{11} & 0 \hline n_j & 0 & 0 \end{vmatrix} \]
    first order binary diffusivity:
    \[ [D_{ij}] = \frac{3\pi}{16} \left( \frac{2k_B T_{ij}}{n\mu_{ij}} \right)^{\frac{1}{2}} \frac{1}{nQ_{ij}^{(1,1)}} \]
    \( m_{ij} = \frac{m_i m_j}{m_i + m_j} \quad T_{ij} = \frac{m_i T_i + m_j T_j}{m_i + m_j} \)
Non-Equilibrium Formulation (cont.)

- Mass and charge diffusion:
  - Self-Consistent Effective Binary Diffusion, SCEBD (Ramshaw & Chang, 1990):
    \[
    \vec{J}_s = -\frac{D_s}{R_s T_s} \vec{G}_s' + y_s \sum_{j} \frac{D_j}{R_j T_j} \vec{G}_j' \quad \vec{G}_s' = \vec{H}_s - \rho_s q_s \left( \vec{E} + \vec{u}_s \times \vec{B} \right) + y_s \vec{J}_q \times \vec{B} \quad \vec{H}_s = p \nabla z_s + (z_e - y_e) \nabla p - \sum_j \left( \beta_{ej} \nabla \ln T_j - \beta_{je} \nabla \ln T_e \right)
    \]
  - Generalized Ohm’s law (consistent with SCEBD):
    \[
    \vec{J}_q = \sigma \left( \vec{E} + \vec{u}_e \times \vec{B} + \frac{\vec{H}_e}{e_n e} - y_e \frac{\vec{J}_q \times \vec{B}}{e_n e} \right) \quad \vec{H}_e = p \nabla z_e + (z_e - y_e) \nabla p - \sum_j \left( \beta_{ej} \nabla \ln T_j - \beta_{je} \nabla \ln T_e \right)
    \]
  - i.e. three-component plasma:
    \[
    \vec{J}_q = \sigma \left( \vec{E} + \vec{u}_e \times \vec{B} + \frac{\nabla p_e}{e_n e} - \frac{\vec{J}_q \times \vec{B}}{\rho_i} - \frac{\vec{J}_a \times \vec{B}}{\rho_i} \right)
    \]

- Chemical rates:
  - Finite rate chemistry:
    \[
    \dot{\rho}^c_s = M_s \sum_{r=1}^{n_s} \left( b_{s,r} - a_{s,r} \right) w_r \quad \dot{w}_r = -k_{f,r} \prod_i \left( \frac{\rho_i}{M_i} \right)^{a_{i,r}} + k_{b,r} \prod_i \left( \frac{\rho_i}{M_i} \right)^{b_{i,r}}
    \]

- Energy exchange:
  - Appleton & Bray, 1964:
    \[
    \dot{Q}_{eh} = \sum_{s=1}^{n_s} \frac{2 k_B}{m_s + m_e} \left( \frac{2 m_s m_e}{m_s + m_e} \right) \vec{v}_{se} (T_e - T_h)
    \]
  - Landau-Teller approx.
    \[
    \dot{Q}_{r-v} = \sum_{s=1}^{n_s} \rho_s \frac{e_{vs} (T) - e_{vs} (T_v)}{\tau_{vs}}
    \]
Direct-Current (DC) Arc Plasma Torch

SG-100 Plasma Spraying Torch

* http://www.praxair.com
### Boundary Conditions

<table>
<thead>
<tr>
<th>Side</th>
<th>$p$</th>
<th>$\mathbf{u}$</th>
<th>$T$</th>
<th>$\phi$</th>
<th>$\mathbf{n}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>$p = p_0$</td>
<td>$\mathbf{u} = \mathbf{u}_m(r)$</td>
<td>$T = T_m$</td>
<td>$\partial_\phi = 0$</td>
<td>$A_r = A_{\phi, r}$</td>
</tr>
<tr>
<td>Cathode</td>
<td>$\partial_\phi \mathbf{n} = 0$</td>
<td>$\mathbf{u}_i = 0$</td>
<td>$T = T_{\text{cathode}}(r)$</td>
<td>$\partial_\phi = 0$</td>
<td>$\partial_\mathbf{A} \mathbf{n} = 0$</td>
</tr>
<tr>
<td>Cathode</td>
<td>$\partial_\phi \mathbf{n} = 0$</td>
<td>$\mathbf{u}_i = 0$</td>
<td>$T = T_{\text{cathode}}(z)$</td>
<td>$-\partial_\phi \mathbf{n} = j_{\text{cathode}}(r)$</td>
<td>$\partial_\mathbf{A} \mathbf{n} = 0$</td>
</tr>
<tr>
<td>Outlet-z</td>
<td>$\partial_\phi \mathbf{n} = 0$</td>
<td>$\partial_\mathbf{r} \mathbf{n} = 0$</td>
<td>$\partial T = 0$</td>
<td>$\partial_\phi = 0$</td>
<td>$A_r = A_{\phi, r}$</td>
</tr>
<tr>
<td>Outlet-r</td>
<td>$p = p_{\text{atm}}$</td>
<td>$\partial_\mathbf{r} \mathbf{n} = 0$</td>
<td>$\partial T = 0$</td>
<td>$\partial_\phi = 0$</td>
<td>$\partial_\mathbf{A} \mathbf{n} = 0$</td>
</tr>
<tr>
<td>Wall</td>
<td>$\partial_\phi \mathbf{n} = 0$</td>
<td>$\mathbf{u}_i = 0$</td>
<td>$T = T_{\text{wall}}$</td>
<td>$\partial_\phi = 0$</td>
<td>$\partial_\mathbf{A} \mathbf{n} = 0$</td>
</tr>
<tr>
<td>Anode</td>
<td>$\partial_\phi \mathbf{n} = 0$</td>
<td>$\mathbf{u}_i = 0$</td>
<td>$-k \partial T \mathbf{n} = h_{\text{wall}}(T - T_{\text{wall}})$</td>
<td>$\phi = 0$</td>
<td>$\partial_\mathbf{A} \mathbf{n} = 0$</td>
</tr>
</tbody>
</table>

~ standard, axisymmetric & constant

- **Sponge Zone** (non-reflecting boundary)

- **Side 1:** inlet
- **Side 2:** cathode
- **Side 3:** cathode tip
- **Side 4:** outlet-z
- **Side 5:** outlet-r
- **Side 6:** wall
- **Side 7:** anode
Not even non-equil. can describe reattachment → **model needed**:

- **high σ in front of anode**
  - if $|E_r| > E_0$ → insert high σ channel where $|E_r|_{\text{max}}$
  - allows attachment movement @ low $T_{\text{anode}}$
  & reattachment process
1. Anode attachment dragged by flow follows an helix around anode surface

2. As arc elongates, $\Delta \varphi \uparrow$ ⇒ arc jumps to form a new attachment

3. New attachment remains, arc is dragged again, starting a new cycle
Takeover Mode - Different Torch Geometries

\[ I = 600 \text{ A, Ar-H}_2 (75-25), 60 \text{ slpm, straight injection} \]

- Larger diameter → smaller reattach. frequency
- Constricted anode → longer arc, smaller freq.
- Smaller diameter → higher reattach. frequency
Electric and Magnetic Potentials & Fields - Jet
Modeling of Instabilities

- Flow, temperature and electromagnetic forcing, i.e. \( u = u_m + u' \)
- Perturbations limited by mesh size \( h \rightarrow \) high resolution required

\[\text{Parabolic Profile, } U_{\text{max}} = 100 \text{ [m/s]}\]

\[\text{Perturbation Function, } f_2 \propto \sqrt{U_2' U_2'}\]

\[\text{Perturbation Velocity Profile, } U_2'\]

\[\text{Total Velocity Profile}\]

- if unstable: small perturbations \( \rightarrow \) macroscopic effects on flow
A Simple Multiscale Problem

1\textsuperscript{st} order ODE: 

\[ y' = 1, \quad y(0) = 0 \]

Solution: 

\[ y = x \]

Perturbed ODE (\( \varepsilon \to 0 \)): 

\[ -\varepsilon y'' + y' = 1, \quad y(0) = 0, \quad y(1) = 0 \]

Solution: 

\[ y = x - \left( \frac{1 - \exp(x/\varepsilon)}{1 - \exp(1/\varepsilon)} \right) \]

![Graph of the 1st order ODE and perturbed ODE with boundary layer indication.]
Multiscale Problems

Why are multiscale problems difficult?

- Any numerical method (i.e. finite differences, volumes, elements, spectral) will fail unless \( \Delta x < O(\varepsilon) \)

Why?

- Smallest scale needs to be resolved. Generally:
  \[
  \Delta x < \text{smallest spatial scale} \quad \& \quad \Delta t < \text{smallest temporal scale}
  \]

- Unmanageable in TADR equations in 3D

Solution:

- Design methods that take into account the effect of the smallest (unsolvable) scales into the large (solvable) scales (dumping the smallest scales also works)