Research Projects in Math Modeling and Numerical Analysis

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Graduate Student Seminar
May 14, 2014

Outline

1. **Electromagnetics**
   - Maxwell's Equations
   - Numerical Analysis
   - Dispersive Media
   - Inverse Problems

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   - Robust Optimization
3. **Magneto-Hydrodynamic (MHD) generator**
   - Model
   - Solution Method
   - Inverse Problem

Acknowledgements

Collaborators

- H. T. Banks (NCSU)
- V. A. Bokil (OSU)
- W. P. Winfree (NASA)

Students

- Karen Barrese and Neel Chugh (REU 2008)
- Anne Marie Milne and Danielle Wedde (REU 2009)
- Erin Bela and Erik Hortsch (REU 2010)
- Megan Armentrout (MS 2011)
- Brian McKenzie (MS 2011)

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H} \qquad \text{(Ampere)}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \text{(Faraday)}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Poisson)}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss)}$$

$\mathbf{E} =$	Electric field vector	$\mathbf{D} =$	Electric flux density
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density
$\rho =$	Electric charge density	$\mathbf{J} =$	Current density

With appropriate initial conditions and boundary conditions.

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$
$$\mathbf{B} = \mu \mathbf{H} + \mathbf{M}$$
$$\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_s$$

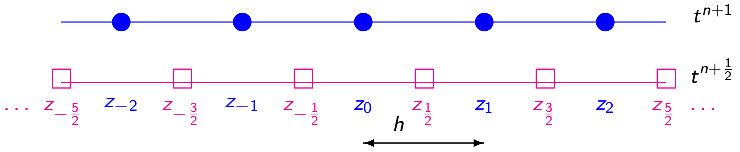
$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Yee Scheme in One Space Dimension

- **Staggered Grids**: The electric field/flux is evaluated on the primary grid in both space and time and the magnetic field/flux is evaluated on the dual grid in space and time.
- The Yee scheme is

$$\frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\mu}\frac{E|_{\ell+1}^{n} - E|_{\ell}^{n}}{\Delta z}$$

$$\frac{E|_{\ell}^{n+1} - E|_{\ell}^{n}}{\Delta t} = -\frac{1}{\epsilon}\frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z}$$



Yee Scheme in One Space Dimension

- This gives an explicit second order accurate scheme in both time and space.

Yee Scheme in One Space Dimension

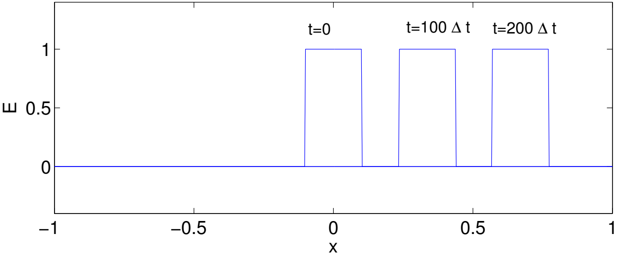
- This gives an explicit second order accurate scheme in both time and space.
- It is conditionally stable with the CFL condition

$$\nu = \frac{c\Delta t}{\Delta z} \leq 1$$

where ν is called the Courant number and $c = 1/\sqrt{\epsilon\mu}$.

Numerical Stability: A Square Wave

- Case $c\Delta t = \Delta z$



Numerical Stability: A Square Wave

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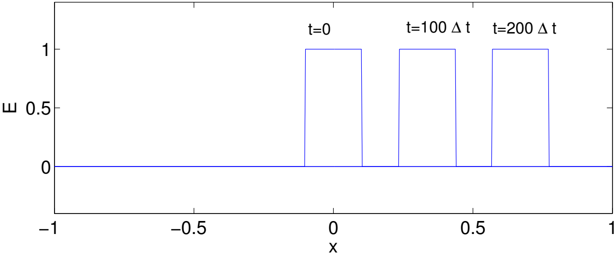
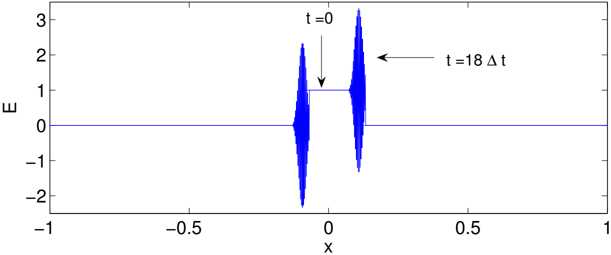
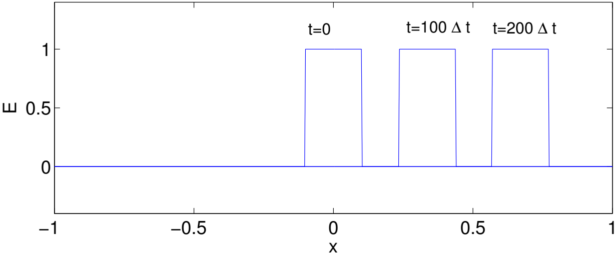


- Case $c\Delta t > \Delta z$

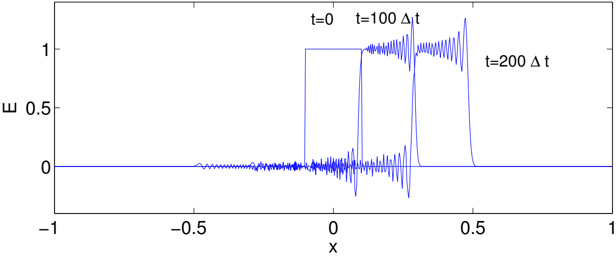


Numerical Dispersion: A Square Wave

- Case $c\Delta t = \Delta z$



- Case $c\Delta t < \Delta z$



Dispersion Error

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- Dispersion error can be reduced by using higher order accurate methods, e.g., $(2, 2M)$ order accurate methods

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Theorem (CFL for $(2, 2M)$ [Bokil-G, 2011])

The method is conditionally stable with CFL condition

$$\nu \left(\sum_{p=1}^{M} \gamma_{2p-1} \right) < 1,$$

$$\gamma_{2p-1} := \sum_{j=p}^{M} \frac{(-1)^{3j-p-2}(j+p-2)![(2M-1)!!]^2 2^{2p-1}}{(2p-1)!(j-p)!(2j-1)(2M-2j)!!(2M+2j-2)!!}$$
$$= \frac{[(2p-3)!!]^2}{(2p-1)!}.$$

Dispersion Error (cont.)

- Mimetic methods adapt free parameters in the scheme to reduce certain errors, e.g., dispersion error [Bokil-G-Gyrya-McGregor, submitted 2014].

Complex permittivity

- We can usually define **P** in terms of a convolution

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).
- In the frequency domain $\hat{\mathbf{D}} = \epsilon\hat{\mathbf{E}} + \hat{\mathbf{g}}\hat{\mathbf{E}} = \epsilon_0\epsilon(\omega)\hat{\mathbf{E}}$, where $\epsilon(\omega)$ is called the complex permittivity.
- $\epsilon(\omega)$ described by the polarization model
- We are interested in ultra-wide bandwidth electromagnetic pulse interrogation of dispersive dielectrics, therefore we want an accurate representation of $\epsilon(\omega)$ over a broad range of frequencies.

Dry skin data

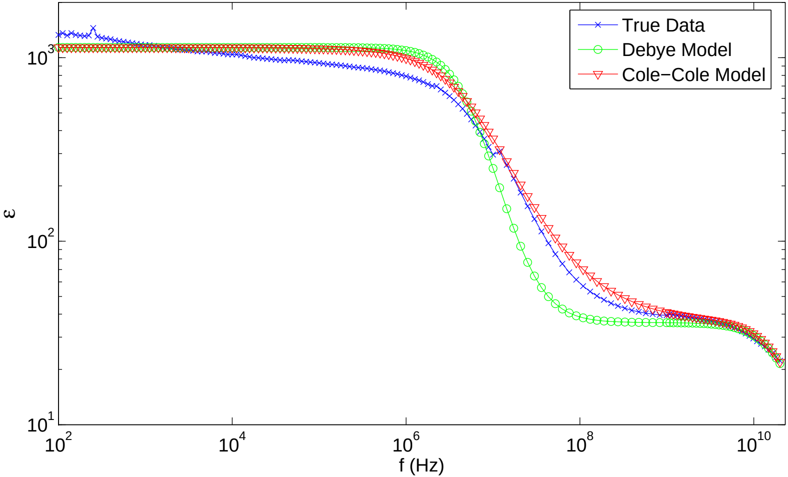

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

- Debye model [1929] $\mathbf{q} = [\epsilon_d, \tau]$

$$g(t,\mathbf{x}) = \epsilon_0\epsilon_d/\tau \quad e^{-t/\tau}$$

$$\text{or} \quad \tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0\epsilon_d\mathbf{E}$$

$$\text{or} \quad \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1+i\omega\tau}$$

with $\epsilon_d := \epsilon_s - \epsilon_\infty$ and τ a relaxation time.

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  with $\epsilon_d := \epsilon_s - \epsilon_\infty$ and τ a relaxation time.
- Cole-Cole model [1936] (heuristic generalization) $\mathbf{q} = [\epsilon_d, \tau, \alpha]$

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1+(i\omega\tau)^{1-\alpha}}$$

Dispersive Media

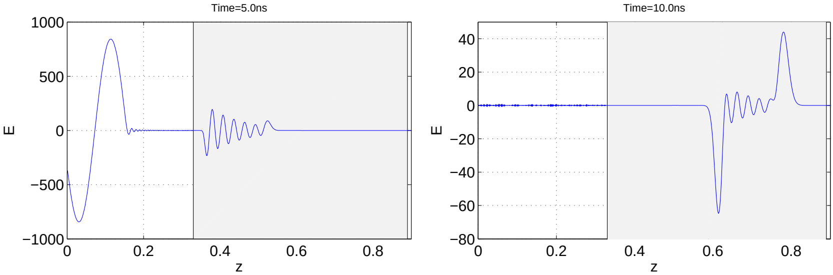

Figure: Debye model simulations.

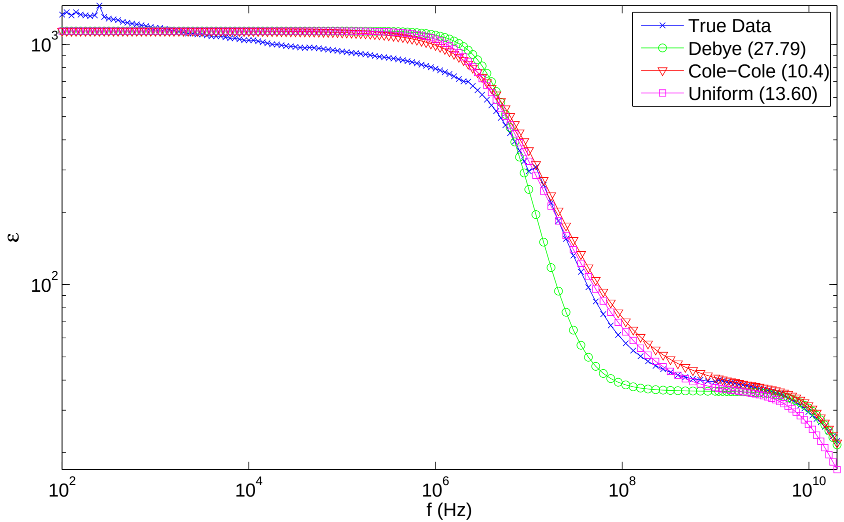

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

Random Polarization

We can define the random polarization $\mathcal{P}(t, \mathbf{x}; \tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d\mathbf{E}$$

where τ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.

The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point $(t, \mathbf{x})$

$$\mathbf{P}(t, \mathbf{x}) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, \mathbf{x}; \tau) f(\tau) d\tau.$$

Polynomial Chaos

Apply Polynomial Chaos method to approximate the random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E, \quad \tau = \tau(\xi) = r\xi + m$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1}$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

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$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

The macroscopic polarization, the expected value of the random polarization at each point (t, x), is simply

$$P(t, x; F) = \alpha_0(t, x).$$

Inverse Problems

Definition

An inverse problem estimates quantities *indirectly* by using measurements of other quantities.

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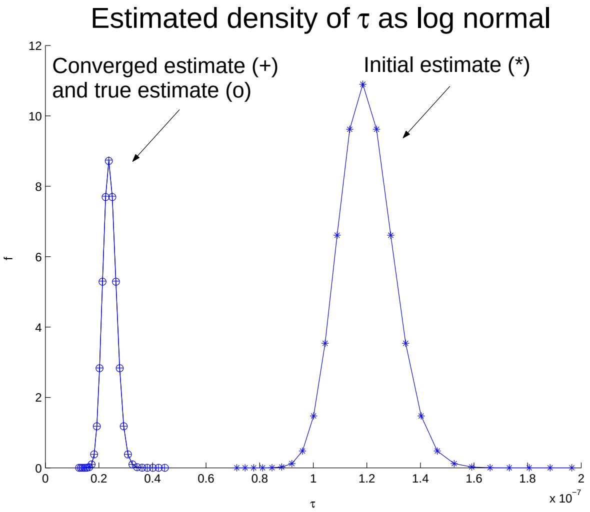
For example, a parameter estimation inverse problem attempts to determine values of a parameter set q given (discrete) observations of (some) state variables.
Examples:

- distance of an object using echo-location (easily invertible)
- amount of oil/water/cave in the ground using RADAR backscatter
- geometry or composition of a defect using measurements of EM fields (CT, MRI, etc.)



Shown are the initial density function, the minimizing density function and the true density function (the latter two being practically identical).

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   - Model
   - Solution Method
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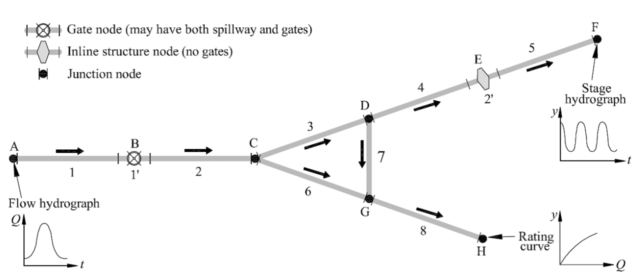
Group Members

- Department of Civil and Construction Engineering
  - Dr. Arturo Leon (PI)
  - Dr. Duan Chen (Post-doc)
  - Mahabub Alam (Ph.D. student)
  - Luis Gomez-Cunya (Ph.D. student)
  - Parnian Hosseini (Ph.D. student)
  - Christopher Gifford-Miears (MS student)
- Department of Mathematics
  - Dr. Nathan Gibson (Co-PI)
  - Dr. Veronika Vasylkivska (Post-doc)
- Department of Mechanical Engineering
  - Dr. Christopher Hoyle (Co-PI)
  - Matthew McIntire (Ph.D. student)

Funded by BPA Technology Innovation Program: "Towards reduction of uncertainty in the operation of reservoir systems"

Simple River System

Consider this simple network system



Unknowns: flow discharge upstream Q_u and downstream Q_d, water surface elevation downstream WSE_d for each reach $i = \overline{1, 8}$.

Simulation of Unsteady Flows

- Most free surface flows are unsteady and nonuniform.
- Unsteady flows in river systems are typically simulated using one-dimensional models.

Saint-Venant equations, PDEs representing conservation of mass and momentum for a control volume:

$$B\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = 0, \quad (1)$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + gA\left(\frac{\partial y}{\partial x} + S_f - S_0\right) = 0, \quad (2)$$

where x is a distance along the channel in the longitudinal direction, t is time, y is a water depth, Q is a flow discharge, B is a width of the channel, g is an accelaration due to gravity, A is a cross-sectional area of the flow, S_f is a friction slope, S_0 is a river bed slope.

Initial and boundary conditions are required to close the system.

Objective and Constraints

The broad context of the problem of interest is a PDEs-constrained optimal control problem with uncertainty. In particular, an objective is expected to be optimized by choices of a control functions.

Let P be a price, and E be a produced hydro-power energy, then $R = P \cdot E$ is a revenue.

Objective: $\max R$,

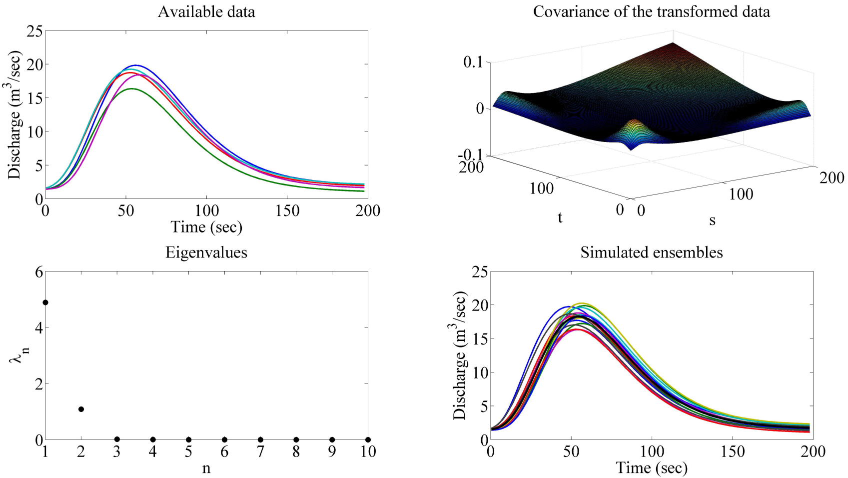
Let Q_t denote a turbine flow, Q_s a spill flow, and S a storage.

Examples of additional constraints:

$$
\begin{aligned}
&0 < Q_t^n < Q_{crit},\\
&0 \leq Q_s^n,\\
&0 < |Q_t^{n+1} + Q_s^{n+1} - Q_t^n - Q_s^n| < \text{Allowed Value},\\
&S_{\min} < S^n < S_{\max}.
\end{aligned}
$$

Numerical Experiments. Stochastic Parametrizations

Experiment 1: 5 predictions



Robust Optimization

The deterministic constrained optimization problem can be formulated as

$$\text{find} \quad \max_q R(q), \tag{3}$$

$$\text{subject to} \quad y(x,t;q) < y_{crit}(x), \tag{4}$$

where q is a control vector.

We assume that price is deterministic and reformulate our problem as follows

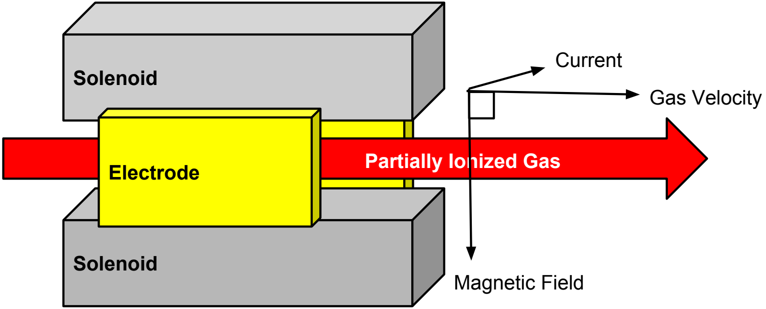
$$\text{find} \quad \max_q \Big(E[R(q)] - \alpha \mathrm{Var}[R(q)] \Big), \tag{5}$$

$$\text{subject to} \quad P(y(x,t;q) < y_{crit}(x)) > R_0, \tag{6}$$

where $\alpha > 0$ is a risk tolerance coefficient, R_0 is a reliability level the decision maker wishes to achieve.

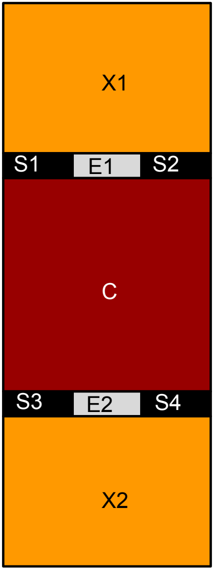
Outline

MHD generator



Funded by National Energy Technology Laboratory Office of Research & Development Fund: "Applying Computational Methods to Determine the Electric Current Densities in a Magnetohydrodynamic Generator Channel from External Magnetic Flux Density Measurements", with Vrushali Bokil (Co-PI)

A slice of simplified generator geometry



- External Casing (Copper?)
- Electrode (Ceramics?)
- Insulating Segment
- Generator Channel

We assume the fluid-electro-magnetic system model by the following system of ten non-linear, partial differential equations.

$$\rho\left(\partial_t - \mathbf{u}\cdot\nabla\right)\mathbf{u} = \mathbf{j}\times\mathbf{b} - \nabla p \qquad \text{Momentum} \quad (7a)$$

$$\rho\partial_t\left(\frac{\mathbf{u}\cdot\mathbf{u}}{2} + U + \frac{\epsilon\mathbf{e}\cdot\mathbf{e}}{2} + \frac{\mathbf{b}\cdot\mathbf{b}}{2\mu}\right) \quad (7b)$$

$$+\rho\mathbf{u}\cdot\nabla\left(\frac{\mathbf{u}\cdot\mathbf{u}}{2} + U\right) = -\nabla\cdot(\mathbf{u}p) - \nabla\cdot\left(\mu^{-1}\mathbf{e}\times\mathbf{b}\right) \qquad \text{Energy} \quad (7c)$$

$$(\partial_t + \mathbf{v}\cdot\nabla)\rho = -\rho\nabla\cdot\mathbf{v} \qquad \text{Mass} \quad (7d)$$

$$\partial_t\epsilon\mathbf{e} + \mathbf{j} = \nabla\times\mu^{-1}\mathbf{b} \qquad \text{Ampere's Law} \quad (7e)$$

$$\partial_t\mathbf{b} = -\nabla\times\mathbf{e} \qquad \text{Faraday's Law} \quad (7f)$$

$$\mathbf{j} = \sigma(\mathbf{e} + \mathbf{u}\times\mathbf{b}) + \frac{\beta}{\sqrt{\mathbf{b}\cdot\mathbf{b}}}\mathbf{j}\times\mathbf{b} \qquad \text{Ohm's Law} \quad (7g)$$

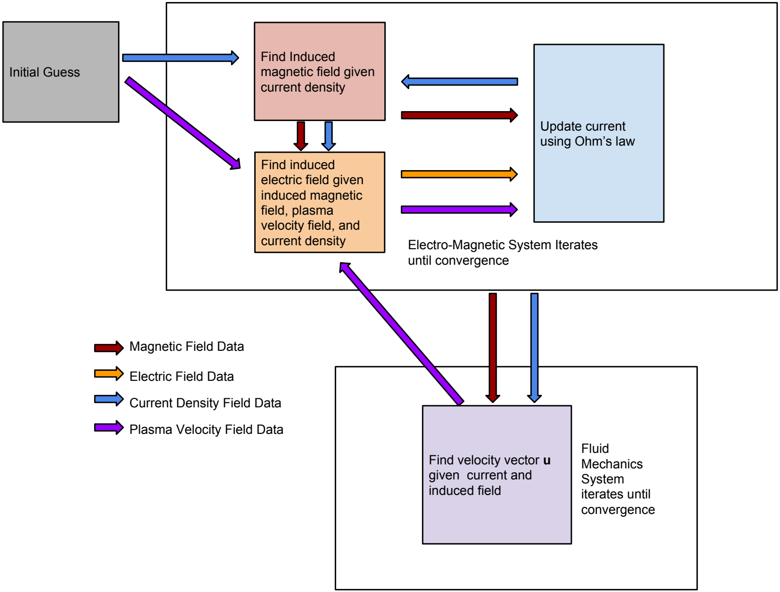
$$\nabla\cdot\epsilon\mathbf{e} = \rho_c \qquad \text{Gauss' Law} \quad (7h)$$

$$\nabla\cdot\mathbf{b} = 0 \qquad \text{Gauss' Law for Magnetism} \quad (7i)$$

With the following variable definitions:

$\mathbf{u}$	gas velocity
p	pressure
ρ	gas density
U	thermal energy
$\mathbf{e}$	electric field
$\mathbf{b}$	magnetic flux density field
$\mathbf{j}$	current density field
ρ_c	charge density
ϵ	electrical permitivity (tensor)
μ	magnetic permeability (tensor)
σ	conductivity (tensor)
β	Hall parameter (tensor)

Fixed Point Approach



Inverse Problem