Computational Models of Exoplanetary Atmospheres

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Outline

Why?

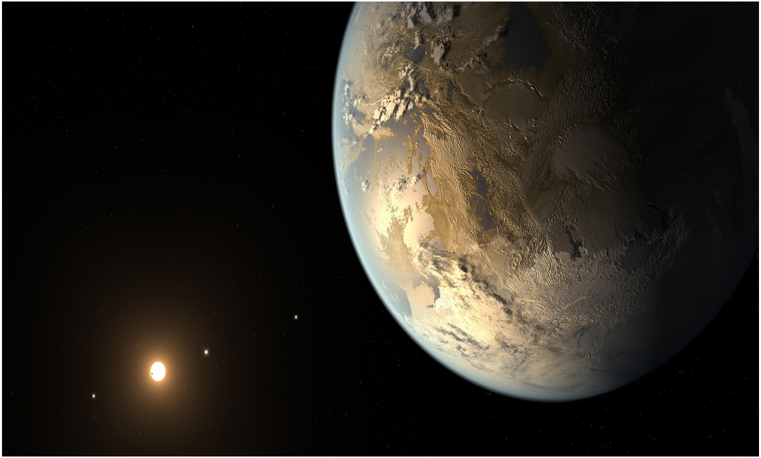


Figure: Artist's depiction of **Kepler-186f**, the first validated Earth-size planet to orbit a distant star in the habitable zone. (https://exoplanets.nasa.gov)

Exoplanets

- Hot Jupiters are a class of gas giant exoplanets that are inferred to be physically similar to Jupiter but that have very short orbital periods.

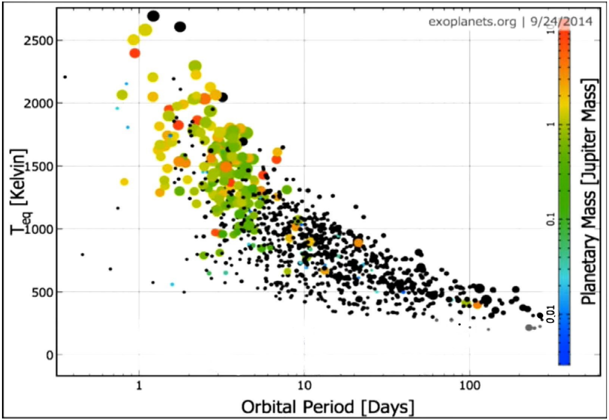


Figure: Survey from Kepler Space Mission of Terrestrial and Gas Planets.

What can we Observe?

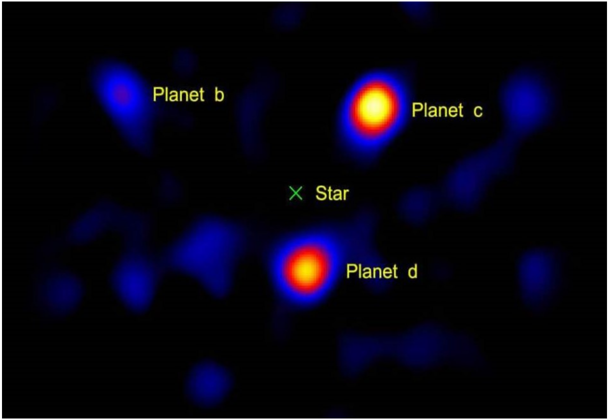
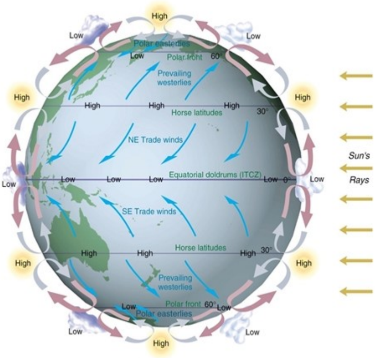


Figure: Three planets orbiting HR8799, 120 light-years away, are thought to be gas giants like Jupiter, but more massive. (NASA/JPL-Caltech/Palomar Observatory).

Atmospheric Dynamics of Earth

- The movement of air through Earth's atmosphere is called wind, and the main cause of Earth's winds is uneven heating by the sun.
- This is a linear model: laminar flow.
- Reality is highly non-linear, turbulent flow.
- Link - Atmospheric Flow



$$\vec{F}_c = -2m\vec{\Omega} \times \vec{v} \qquad (1)$$

What Physical Parameters that Influence the Atmospheric Dynamics of Hot Jupiters?

- Consider Jupiter in our own solar system for reference.

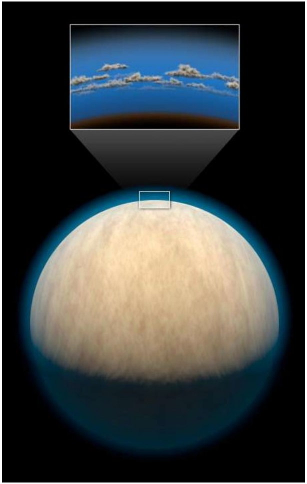
- Angular velocity
- Magnetic fields
- Magnetic diffusivity
- Molecular viscosity
- Rayleigh drag
- Solar irradiation

How Does One Model Exoplanetary Atmospheres?

- **Analytical Models:** Explains things in terms of equation. If a solution exists then great, but that often is not the case.
- **Computation Models:** Requires running simulations on different aspects of an analytical model using different equations and studying the results. Extremely difficult to distinguish results.

Purpose

- The study of exoplanetary atmospheres is a vast and complex field.
- The purpose of this seminar is to introduce you to a new field of research and demonstrate the necessary requirements to create a model to study an intricate object such as a Hot Jupiter.



Outline

Analytical Models

- Analyzed the stability criterion of 12 different 1D models of varying complexity.
- Models[1] governed by set of 5, highly non-linear PDE's.

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\vec{V}) = Q \tag{2}$$

$$\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} = -g\nabla h + \nu \nabla^2 \vec{V} - \frac{\vec{V}}{t_{drag}} - 2\vec{\Omega} \times \vec{V} + \frac{\vec{B} \cdot \nabla \vec{B}}{4\pi\rho} \tag{3}$$

$$\frac{\partial \vec{B}}{\partial t} = \nabla \times \left(\vec{V} \times \vec{B}\right) + \eta \nabla^2 \vec{B} \tag{4}$$

[1] [Heng and Workman 2014]

Outline

Numerical Models

To learn the basics of creating numerical models, the text "Computational Fluid Dynamics: The Basics with Applications", by John D. Anderson[2] was heavily utilized in this research.

- Simulate the fluid flow variables: (ρ, V, T, p).
- Run the simulation by marching forward in time towards an equilibrium state.

$$\frac{\partial(\rho, V, T, p)}{\partial t} = 0 \tag{5}$$

- How will the program evaluate spatial and temporal derivatives?

[2] [John D. Anderson 1995]

Governing Equations

- Euler Equations are a reduced form of the Navier Stokes Equations.
- The governing equations for an inviscid flow, in conservation form, are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V}\right) = 0 \tag{6}$$

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot \left(\rho u \vec{V}\right) = -\frac{\partial p}{\partial x} + \rho f_x \tag{7}$$

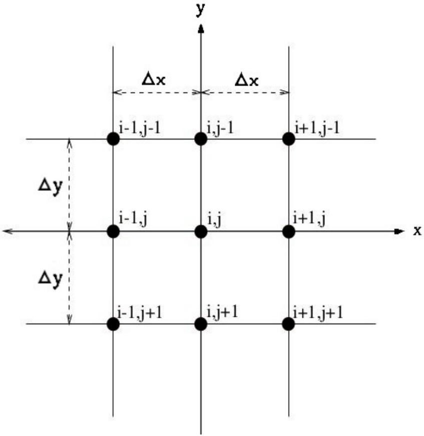
$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot \left(\rho v \vec{V}\right) = -\frac{\partial p}{\partial y} + \rho f_y \tag{8}$$

$$\frac{\partial(\rho w)}{\partial t} + \nabla \cdot \left(\rho w \vec{V}\right) = -\frac{\partial p}{\partial z} + \rho f_z \tag{9}$$

$$\frac{\partial}{\partial t}\left[\rho\left(e + \frac{V^2}{2}\right)\right] + \nabla \cdot \left[\rho\left(e + \frac{V^2}{2}\right)\vec{V}\right] = \rho \dot{q} - \nabla \cdot \left(p\vec{V}\right) + \rho \vec{f} \cdot \vec{V}. \tag{10}$$

Continuous to Discrete Domain

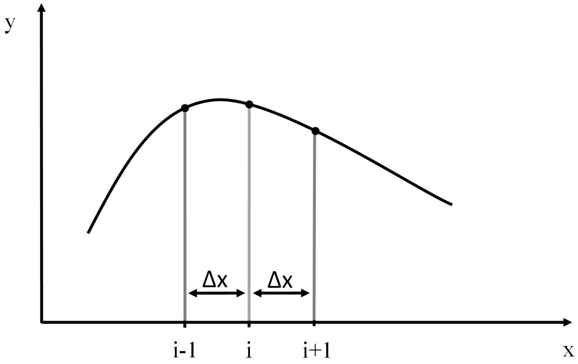
- Discretization is the process of transferring continuous functions, variables, and equations into discrete counterparts.
- Numerical domain is discretized into a finite set of control volumes or cells. The discretized domain is called the "grid".



Finite Difference

Interested in constructing $f(x, t + \Delta t)$ from $\frac{\mathrm{d}f(x,t)}{\mathrm{d}x}$ numerically.

- Need to evaluate $\frac{\mathrm{d}f(x,t)}{\mathrm{d}x}$ numerically.
- Goal is to replace spatial derivatives with a suitable algebraic difference quotient.



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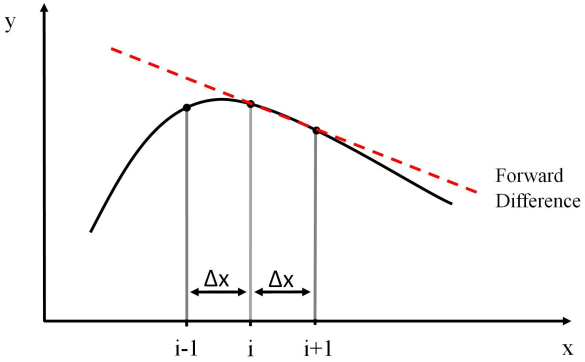

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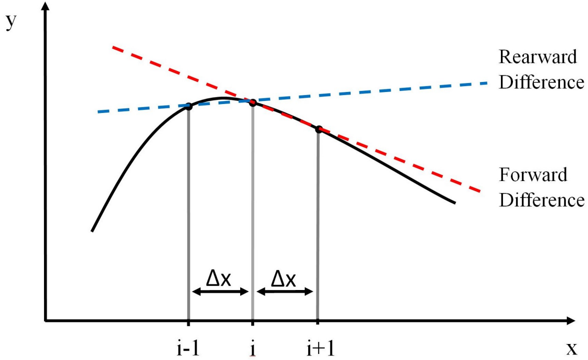

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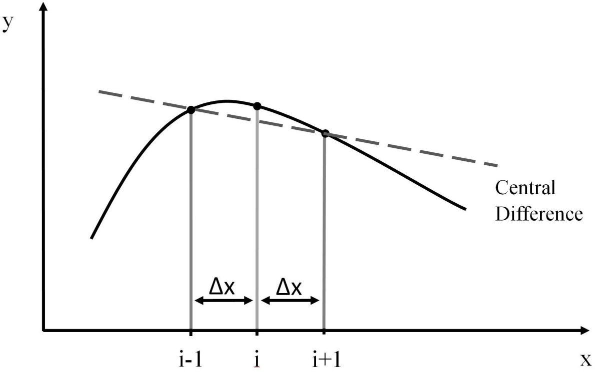

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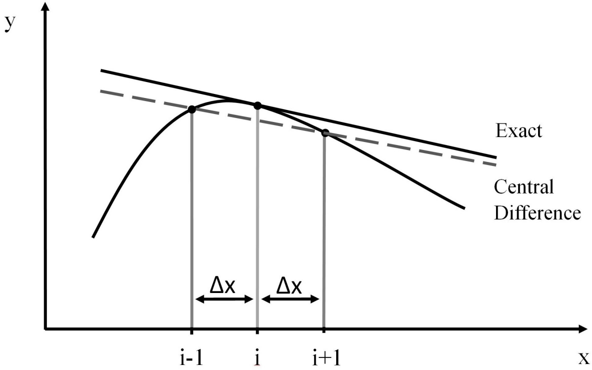

Forward Difference

- Consider the flow field variable $u_{i,j}$ and formulate an expression for the spatial derivative at location (i, j).
- Then, $u_{i+1,j}$ can be expressed in terms of a Taylor series expanded about point (i, j).

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots \quad (11)$$

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$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j} - u_{i,j}}{\Delta x}}_{\text{Forward-difference}} \underbrace{- \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{\Delta x}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^2}{6} + \cdots}_{\text{Truncation error}} \tag{12}$$

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$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{13}$$

Rearward Difference

- Then u at location $(i-1,j)$ can be expressed in terms of a Taylor series about the point (i,j).

$$u_{i-1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j}(-\Delta x) + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(-\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(-\Delta x)^3}{6} + \cdots \quad (14)$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i,j}-u_{i-1,j}}{\Delta x}}_{\text{Rearward-difference}} \underbrace{- \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{\Delta x}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^2}{6} + \cdots}_{\text{Truncation error}} \quad (15)$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j}-u_{i-1,j}}{\Delta x} + O(\Delta x) \quad (16)$$

2nd Order Central Difference

- Central difference quotient is formulated by subtracting the rearward Taylor series expansion, Eq(14), from the forward Taylor series expansion, Eq(11).

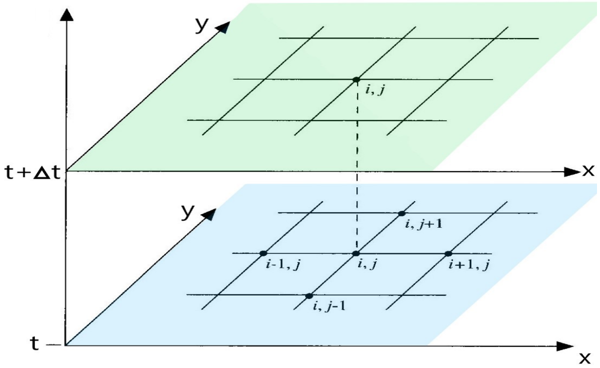
$$u_{i+1,j} - u_{i-1,j} = 2\left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + 2\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{6} + \cdots \tag{17}$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}}_{\text{Central-difference}} \underbrace{- 2\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^2}{6} + \cdots}_{\text{Truncation error}} \tag{18}$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x^2) \tag{19}$$

Explicit Approaches

- Assume flow field variables, ρ, V, T, p, are known at time t and proceed to calculate the flow field variables at time $t + \Delta t$.



MacCormack Technique

- The MacCormack technique is an explicit finite difference technique which is second order accurate in both space and time.
- This technique uses a predictor-corrector scheme to reduce the number of computations while retaining its accuracy.

$$\rho_i^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_i^t \Delta t + \left(\frac{\partial^2 \rho}{\partial t^2}\right)_i^t \frac{(\Delta t)^2}{2} + \cdots \tag{20}$$

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$$\rho_i^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_{av} \Delta t \tag{21}$$

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$$\rho_i^{t+\Delta t} = \rho_i^t + \frac{1}{2}\left[\underbrace{\left(\frac{\partial \rho}{\partial t}\right)_i^t}_{\text{Predictor}} + \underbrace{\left(\overline{\frac{\partial \rho}{\partial t}}\right)_i^{t+\Delta t}}_{\text{Corrector}}\right] \Delta t \tag{22}$$

Outline

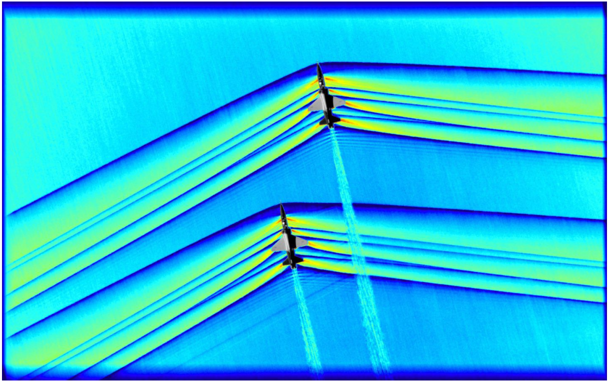
Computational Fluid Dynamics (CFD)

- Computational fluid dynamics is a branch of fluid mechanics that uses numerical analysis and data structures to analyze and solve fluid flow problems.
- Analyzed three numerical flow problems where the governing equations and initial conditions were given by Anderson.[3]
- Nozzle Flow: Predictable results with many engineering applications.
  - Conservation vs Non-Conservation Form
- Shock Capturing: Test the limits of the program with atmospheric application.

[3] [John D. Anderson 1995]

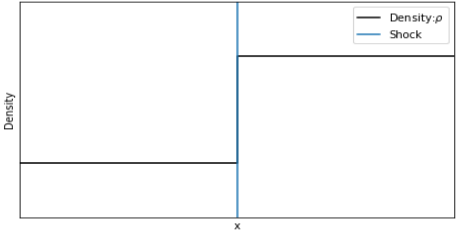
Shock Wave - Shock Front

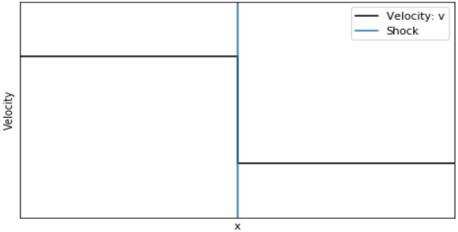
- When an object moves faster than the information can propagate into the surrounding fluid, then the fluid near the disturbance cannot react or "get out of the way" as the disturbance arrives.



Conserved and Non-Conserved Quantities

Non-Conservative Form: Consider the primitive variables, ρ, v.





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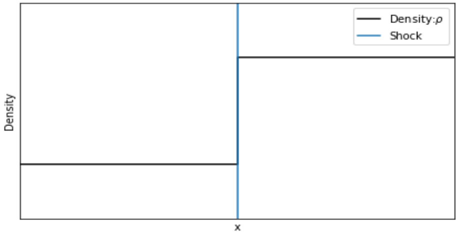
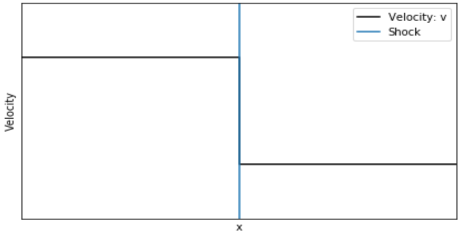
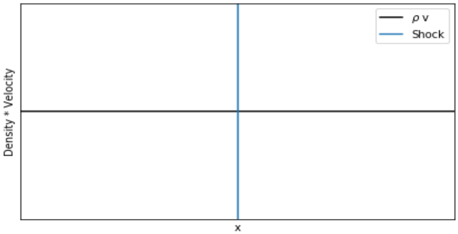


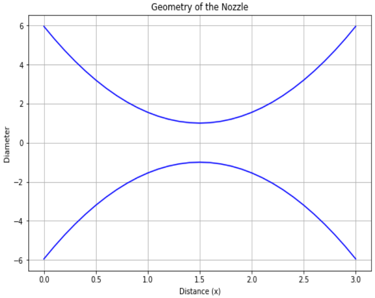


Conservative Form: Consider the quantity mass flow rate: $\rho_1 v_1 = \rho_2 v_2$.



1D Subsonic-Supersonic Isentropic Nozzle Flow

- Implemented a second order, central difference MacCormack technique to solve for steady state solution.
- First analyze nozzle flow with primitive variables and then non-primitive.



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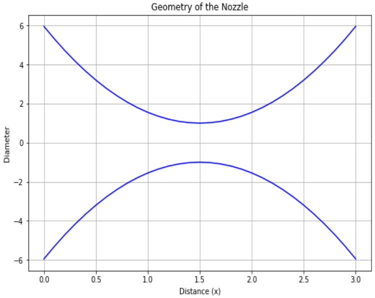
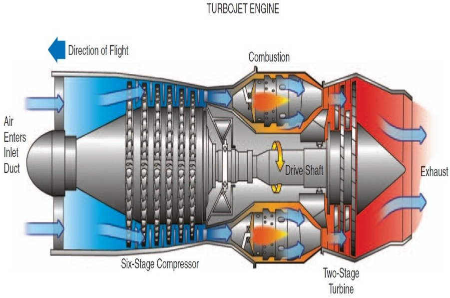




Non-Conservation Form of the Governing Equations

For Ideal Gas, $e = c_v T$, and $p = \rho R T$. For water, $\gamma = \frac{c_p}{c_v} = 1.4$.

- Continuity equation

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial V}{\partial x} - \rho V \frac{\partial (lnA)}{\partial x} - V \frac{\partial \rho}{\partial x} \tag{23}$$

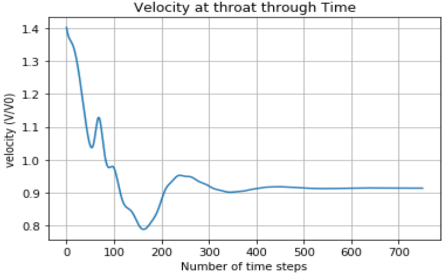
- Momentum equation

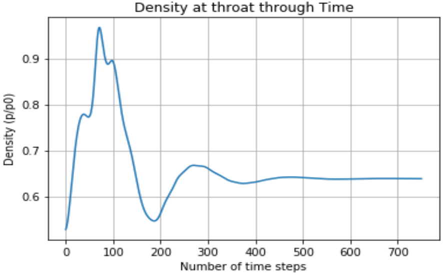
$$\frac{\partial V}{\partial t} = -V \frac{\partial V}{\partial x} - \frac{1}{\gamma}\left(\frac{\partial T}{\partial x} + \frac{T}{\rho}\frac{\partial \rho}{\partial x}\right) \tag{24}$$

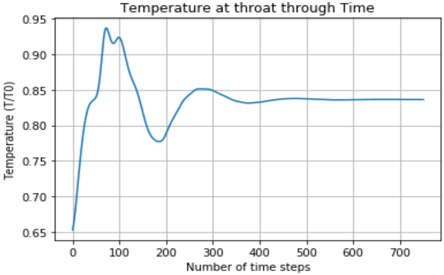
- Energy equation

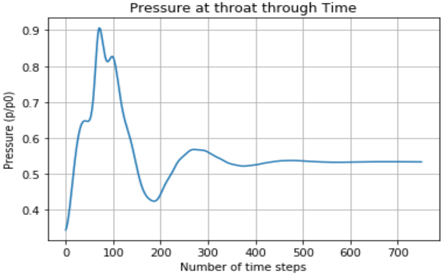
$$\frac{\partial T}{\partial t} = -V \frac{\partial T}{\partial x} - (\gamma - 1) T \left[\frac{\partial V}{\partial x} + V \frac{\partial (lnA)}{\partial x}\right] \tag{25}$$

Primitive Variables at “Throat” of the Nozzle



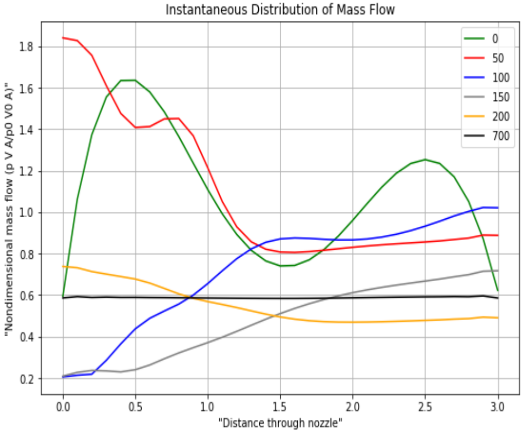






Mass Flow Distribution

- Mass flow is the movement of mass through a pressure gradient.
- Mass Flow: $\rho VA = 0.579$ at steady state.



1D Subsonic-Supersonic Nozzle Flow - Conservation Form

- The governing equations must first be adapted into conservation form.
- Conservation Form Reads:

$$\boxed{\text{Time Rate of Change of Quantities}} + \boxed{\text{Flux of Quantities}} = \boxed{\textit{Source/Sink}}$$

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$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = J \tag{26}$$

- The terms U, F, and J are column vectors where U is the solution vector, F is the flux vector, and J represents the source terms.

Subsonic-Supersonic Nozzle - Conservation Form

- Governing Equation are Encoded into Conservation Form.
- Continuity equation

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho A V)}{\partial x} = 0 \tag{27}$$

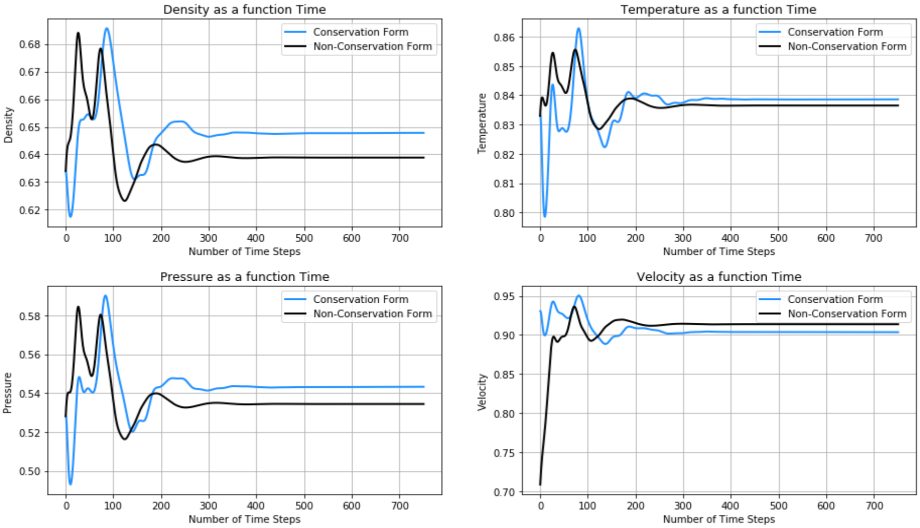
- Momentum equation

$$\frac{\partial(\rho A V)}{\partial t} + \frac{\partial\left[\rho A V^2 + (1/\gamma) p A\right]}{\partial x} = \frac{1}{\gamma} p \frac{\partial A}{\partial x} \tag{28}$$

- Energy equation

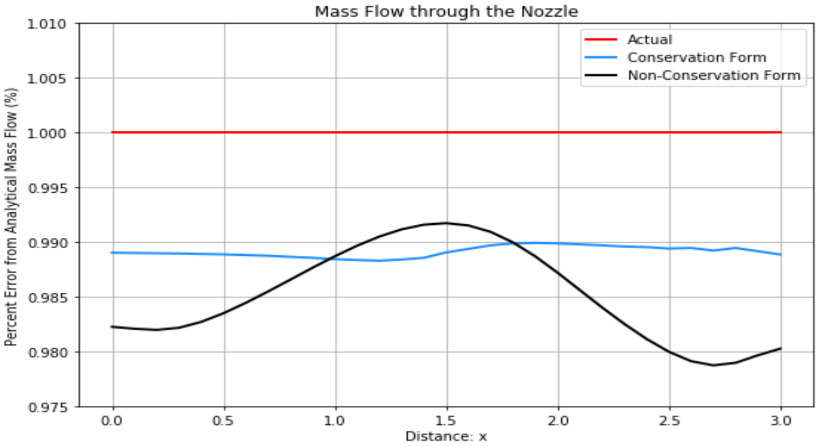
$$\frac{\partial\left[\rho\left(\frac{e}{\gamma-1} + \frac{\gamma}{2} V^2\right) A\right]}{\partial t} + \frac{\partial\left[\rho\left(\frac{e}{\gamma-1} + \frac{\gamma}{2} V^2\right) V A + p A V\right]}{\partial x} = 0 \tag{29}$$

Conservation vs. Non-Conservation Primitive Variables



Percent Error In Mass Flow

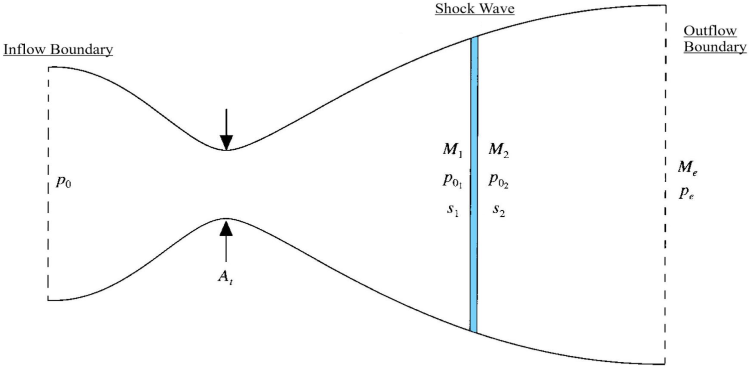
Actual value provided by analytical techniques from Anderson.[4]



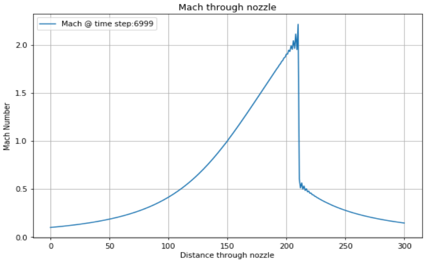
[4] [John D. Anderson 1995]

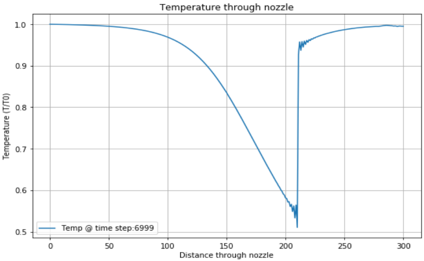
1D Nozzle with Shock Capturing

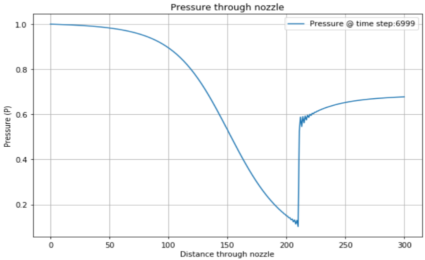
- Now consider a nozzle flow model with shock capturing.
- Ensure the existence of a shock by setting a constant pressure at the exit boundary.

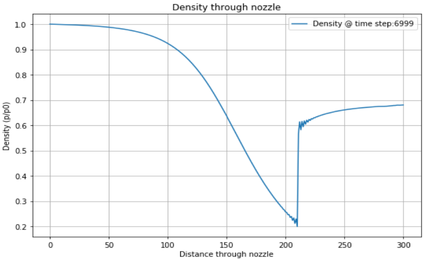


Plots of Decoded Primitive Variables

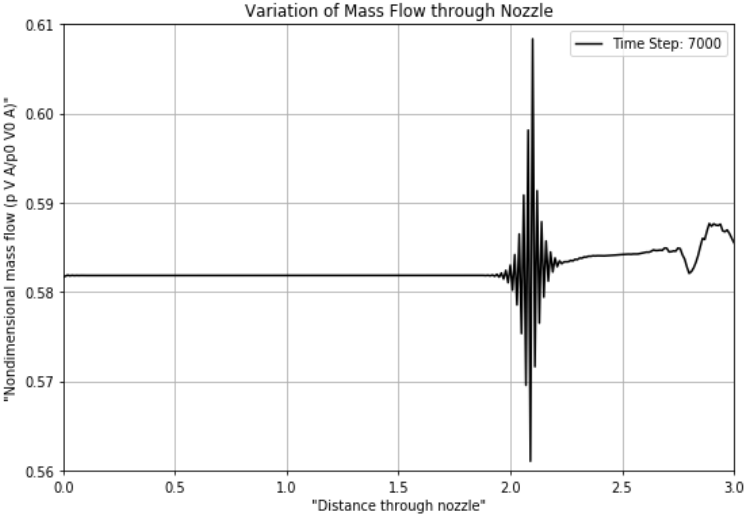








Mass Flow across Shock Wave



Outline

Hydrodynamic Free System

- Using the governing equations provided by Heng and Workman[5], I wrote a program to numerically simulate an atmospheric flow model.
- Implemented a basic equatorial β-plane approximation to capture the essence of being near the equator on a sphere.

$$\frac{\partial h}{\partial t} = -\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} \tag{30}$$

$$\frac{\partial v_x}{\partial t} = -\frac{\partial h}{\partial x} + y v_y \tag{31}$$

$$\frac{\partial v_y}{\partial t} = -\frac{\partial h}{\partial y} - y v_x \tag{32}$$

[5] [Heng and Workman 2014]

Vector Field Simulation

Play/Pause | Reset

Height of Fluid Simulation

Play/Pause Reset

Outline

Conclusion

- What did we learn from this project?
- Why was this research project important?

Final Thoughts

- Produced 5 different simulation programs that open to the public; "https://bitbucket.org/joshlindsey/python-fluid-solver/src/master/".
- ▸ Link - Fluid Simulation Programs
- Lastly, I would like to thank my research advisor, Dr. Workman, for all of his help in this project.

Closing

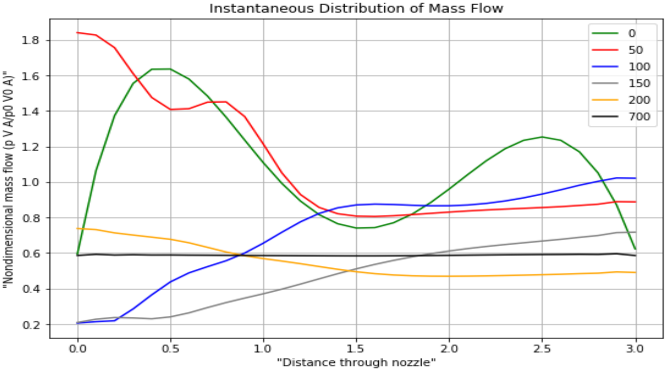
- Thank you for your time.
- Do you have any questions?

Heng and Workman, *Analytical Models of Exoplanetary Atmospheres. Atmospheric Dynamics via The Shallow Water System*. 2014.

John D. Anderson, *Computational Fluid Dynamics: The Basics with Applications*. 1995.

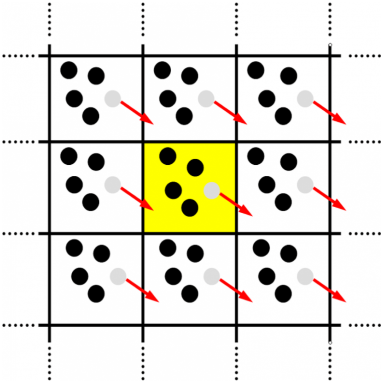
Mass Flow Distribution

- Mass Flow is the movement of mass through a pressure gradient.
- Mass Flow: $\rho VA = 0.579$ at steady state. Mass Flow.gif



Boundary Conditions

- Implement periodic boundary conditions.
- Computational domain is colored in yellow, white spaces are "ghost zones".



Calculation of Time Step

- For stability, the numerical domain must include all the analytical domain.
- C is the Courant number; the stability analysis requires that $C \leq 1$ for an explicit numerical solution to be stable.

$$\Delta t = C \frac{\Delta x}{\sqrt{V_s^2 + V_f^2}} \tag{33}$$

- Calculate $(\Delta t)_i^t$ at all the grid points, $i = 1$ to $i = N$, and choose the minimum value.

$$\Delta t = minimum(\Delta t_1^t, \Delta t_2^t, ..., \Delta t_N^t) \tag{34}$$

Initial and Boundary Conditions

- Boundary conditions are determined by the type of governing equations.
- Inflow Boundary: From the characteristic lines at the inflow boundary, one variable must be specified and one must be allowed to float.

$$\begin{aligned} V_1 =& 2V_2 - V_3 \\ \rho_1 =& 1 \\ T_1 =& 1 \end{aligned} \tag{35}$$

- Outflow Boundary: Both characteristic lines are propagating with the flow at the outflow and all variables are allowed to float.

$$\begin{aligned} V_N =& 2V_{N-1} - V_{N-2} \\ \rho_N =& 2\rho_{N-1} - \rho_{N-2} \\ T_N =& 2T_{N-1} - T_{N-2} \end{aligned} \tag{36}$$

How can we study Exoplanets?

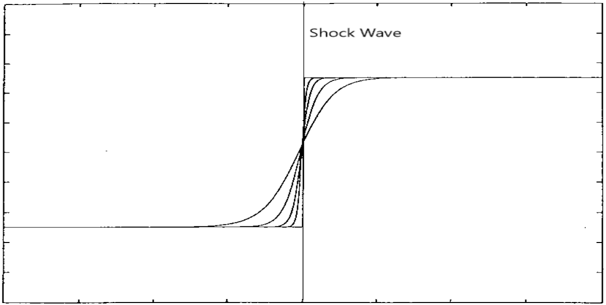
- Due to vast distances of space, our current technology simply can not provide sufficient observational data on terrestrial exoplanets.
- If Astronomers can not study exoplanets directly, then the challenge falls upon the Physicists.

$$\boxed{\text{Astronomers/Observations}} \longrightarrow \boxed{\text{Comp. Physicists/Models}}$$

- Model that which is easiest to observe first so that we can be confident in our models when we try to model that which is difficult to observe.
- Observations

Artificial Viscosity

- There is a numerical phenomena in CFD where dispersion and dissipation terms can occur in the truncation error.
- In addition, artificial viscosity can disperse the shock to make it easier for computations.



MacCormack Technique

- The MacCormack technique is an explicit finite difference technique which is second order accurate in both space and time.
- Assume that the flow field at each grid point is known at time t and proceed to calculate the flow field variables at time $t + \Delta t$.

$$\frac{\partial \rho}{\partial t} = -\left(\rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x}\right) \tag{37}$$

$$\frac{\partial u}{\partial t} = -\left(u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x}\right) \tag{38}$$

$$\frac{\partial e}{\partial t} = -\left(u \frac{\partial e}{\partial x} + \frac{p}{\rho} \frac{\partial u}{\partial x}\right) \tag{39}$$

McCormick Algorithm

- Most algorithms are predicated on a Taylor series expansion in time.
- The McCormick technique uses a predictor-corrector scheme to reduce the number of computations while retaining its accuracy.

$$\rho_i^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_i^t \Delta t + \left(\frac{\partial^2 \rho}{\partial t^2}\right)_i^t \frac{(\Delta t)^2}{2} + \cdots \tag{40}$$

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$$\rho_i^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_{av} \Delta t \tag{41}$$

Predictor Step

- Replace the spatial derivatives with forward differences. Note that all flow field variables at time t are known.

$$\left(\frac{\partial \rho}{\partial t}\right)_i^t = -\left(\rho_i^t \frac{u_{i+1}^t - u_i^t}{\Delta x} + u_i^t \frac{\rho_{i+1}^t - \rho_i^t}{\Delta x}\right) \tag{42}$$

- Obtain a *predicted* value of density $(\overline{\rho})^{t+\Delta t}$ from the first two terms of Taylor series.

$$(\overline{\rho})^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_i^t \Delta t \tag{43}$$

Corrector Step

- Then obtain a *corrected* value of the time derivative at time $t + \Delta t$.

$$\left(\overline{\frac{\partial \rho}{\partial t}}\right)_i^{t+\Delta t} = -\left[(\overline{\rho})_i^{t+\Delta t} \frac{(\overline{u})_i^{t+\Delta t} - (\overline{u})_{i-1}^{t+\Delta t}}{\Delta x} + (\overline{u})_i^{t+\Delta t} \frac{(\overline{\rho})_i^{t+\Delta t} - (\overline{\rho})_{i-1}^{t+\Delta t}}{\Delta x}\right].$$

- The average value of the time derivative is the mean of the *predicted* and *corrected* time derivatives.

$$\left(\frac{\partial \rho}{\partial t}\right)_{av} = \frac{1}{2}\left[\underbrace{\left(\frac{\partial \rho}{\partial t}\right)_i^t}_{\text{Predictor}} + \underbrace{\left(\overline{\frac{\partial \rho}{\partial t}}\right)_i^{t+\Delta t}}_{\text{Corrector}}\right] \tag{44}$$

McCormick Technique

- This algorithm can be applied to solve for all of the flow field variables.
- This algorithm may be adapted to any set of governing equations following an explicit approach.

$$\rho_i^{t+\Delta t} = \rho_i^t + \left(\frac{\partial \rho}{\partial t}\right)_{av} \Delta t \tag{45}$$

$$u_i^{t+\Delta t} = u_i^t + \left(\frac{\partial u}{\partial t}\right)_{av} \Delta t \tag{46}$$

$$e_i^{t+\Delta t} = e_i^t + \left(\frac{\partial e}{\partial t}\right)_{av} \Delta t \tag{47}$$