Numerical Methods for Calculating Planetary Outflow Profiles with Critical Points

Hans De Sterck

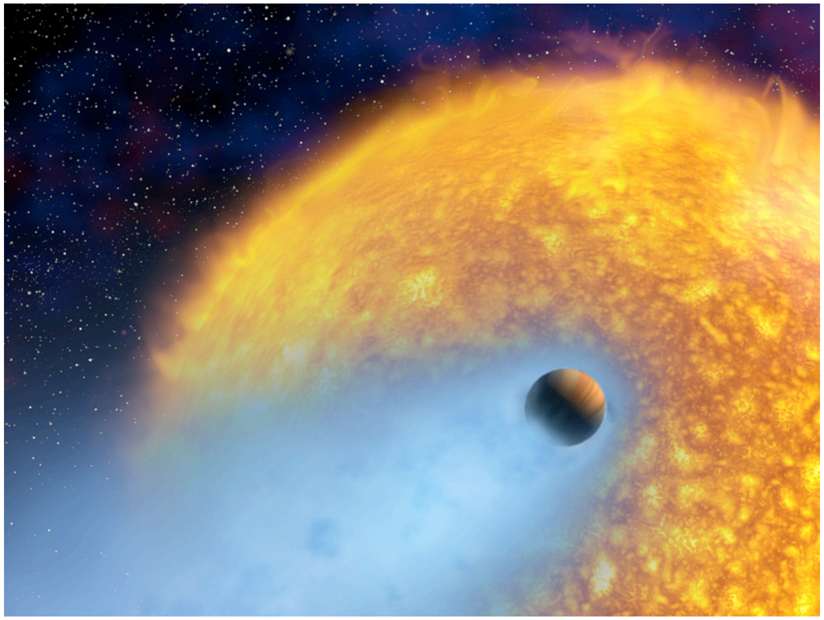
Department of Applied Mathematics, University of Waterloo, Ontario, Canada

University of Waterloo

CPA, July 2007

1. Supersonic gas escape from extrasolar planets

- http://exoplanet.eu
- 173 extrasolar planets known, as of June 2006
- 236 extrasolar planets known, as of May 2007
- 241 extrasolar planets known, as of June 2007!
- 26 multiple planet systems

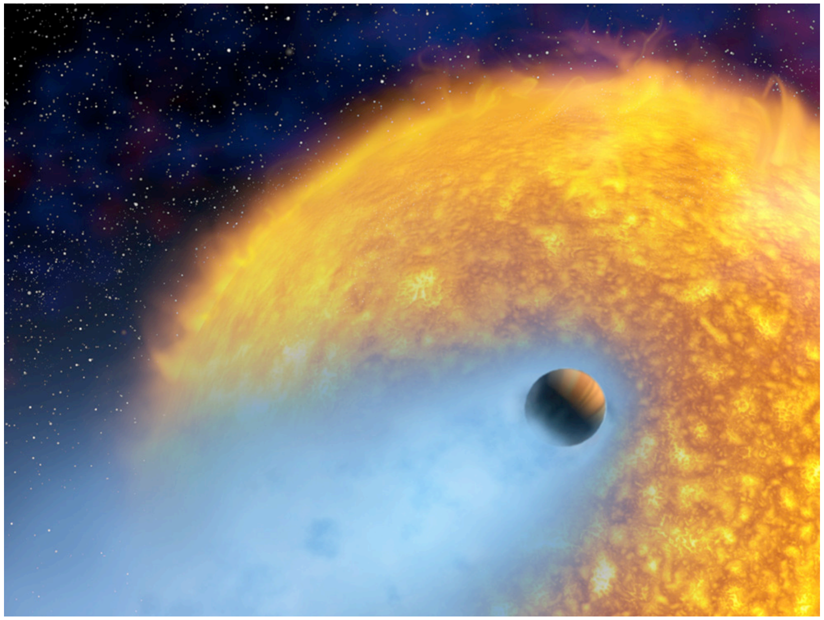


University of Waterloo

CPA, July 2007
hdesterck@uwaterloo.ca

Supersonic gas escape from extrasolar planets

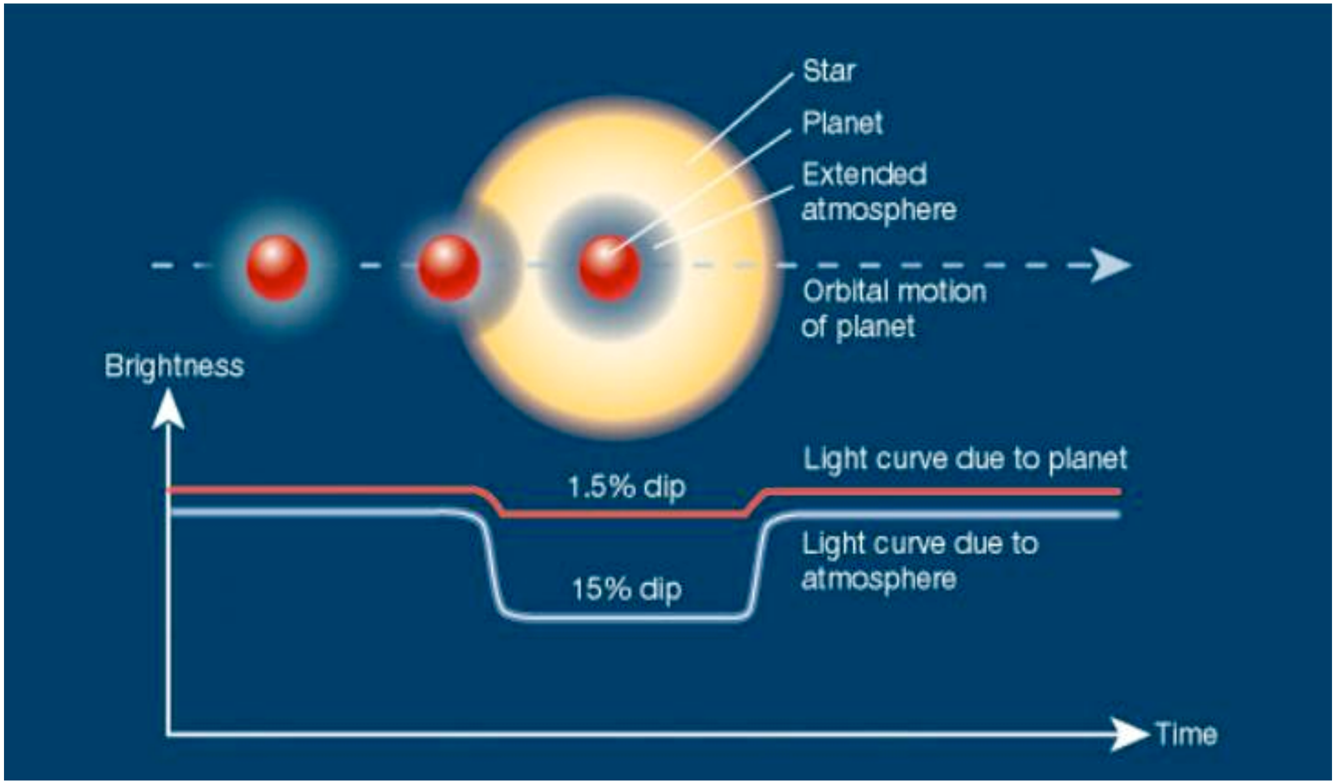
- many exoplanets are gas giants ("hot Jupiters")
- many orbit very close to star (~0.05 AU)
- hypothesis: strong irradiation leads to supersonic hydrogen escape



University of Waterloo

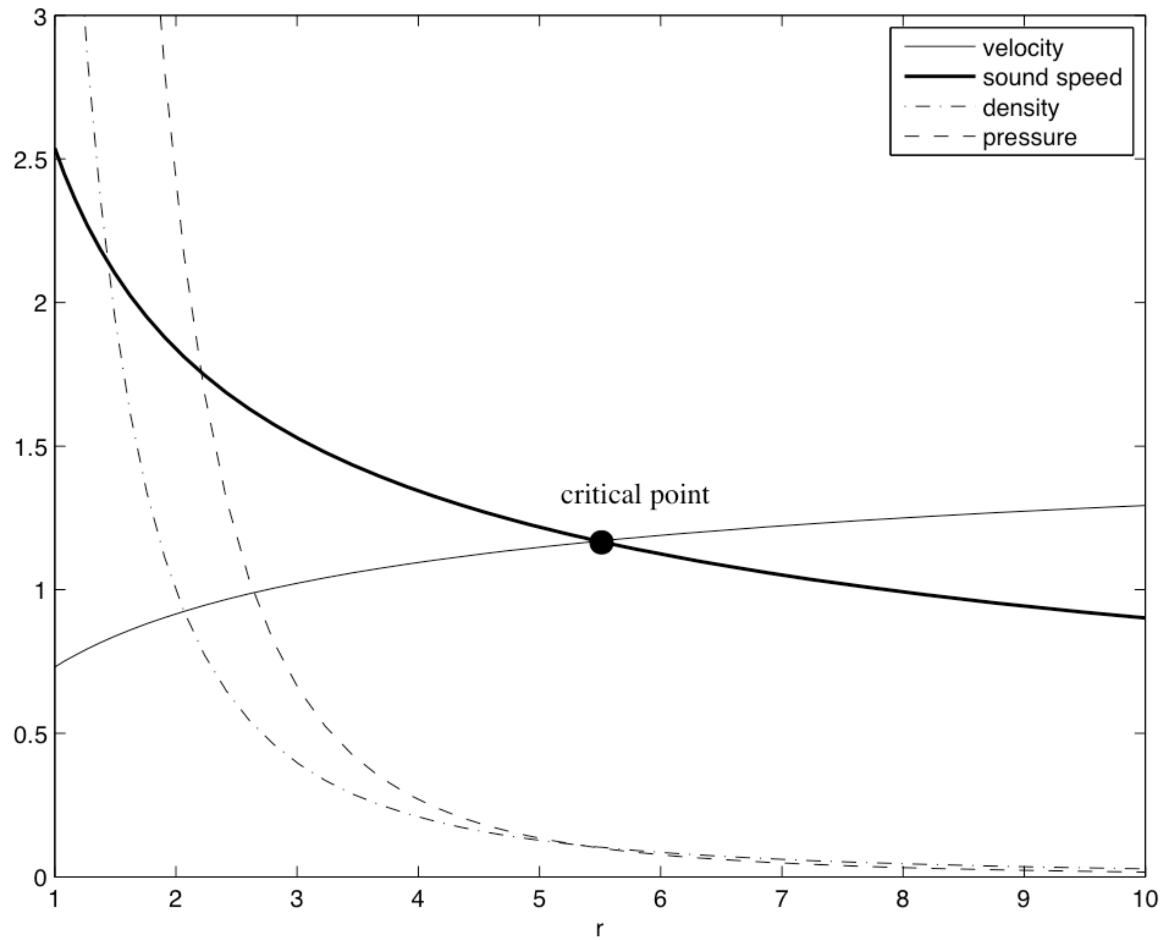
CPA, July 2007
hdesterck@uwaterloo.ca

Example: HD209458 (Vidal-Madjar 2003)



- 0.67 Jupiter masses, 0.05 AU, transiting
- hydrogen atmosphere and escape observed
- question: what is the mass loss rate? long-time stability of the planet? $\Rightarrow$ solve Euler equations!

Transonic radial outflow solution



subsonic ⇒|⇐ supersonic

CPA, July 2007
hdesterck@uwaterloo.ca

University of Waterloo

Euler equations

- radial outflow from extrasolar planet

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho\, r^2 \\ \rho\, u\, r^2 \\ (\frac{p}{\gamma-1} + \frac{\rho\, u^2}{2})\, r^2 \end{bmatrix} + \frac{\partial}{\partial r}\begin{bmatrix} \rho\, u\, r^2 \\ \rho\, u^2\, r^2 + p\, r^2 \\ (\frac{\gamma\, p}{\gamma-1} + \frac{\rho\, u^2}{2})\, u\, r^2 \end{bmatrix}$$

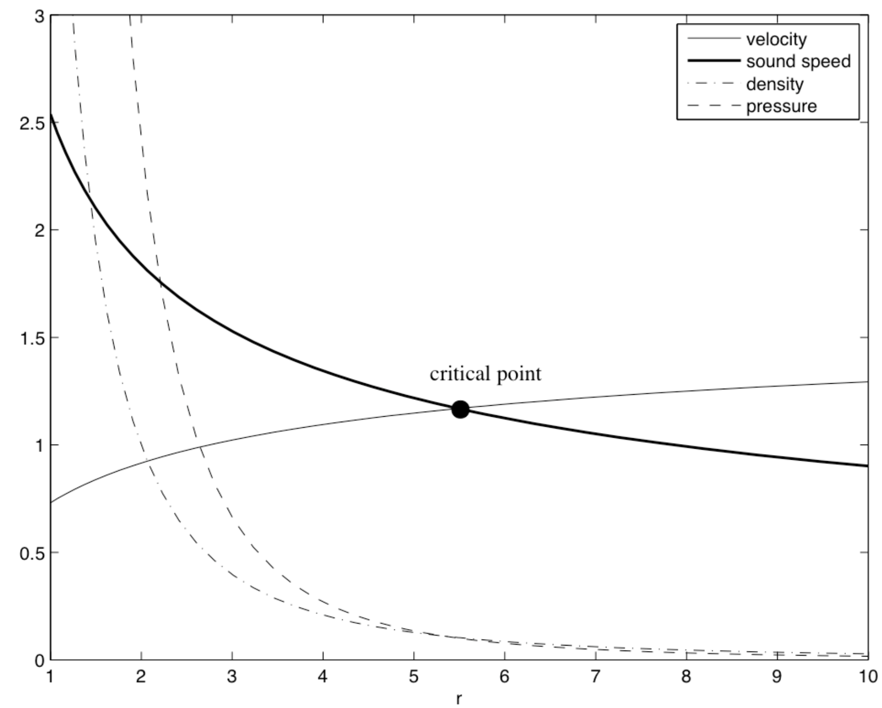
$$= \begin{bmatrix} 0 \\ -\rho G M + 2\, p\, r \\ -\rho G M\, u + q_{heat}\, r^2 \end{bmatrix}$$

Transonic radial outflow solution: problem definition

- goal: given density and pressure at lower boundary, calculate steady solution profile

$$\rho(r), u(r), p(r)$$

- output of interest:
  - o mass flux (mass/time) (how fast does the planet evaporate?)
  - o location of critical point



2. Simulation by time marching

- Euler Equations are conservation law

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial r} = S(U)$$

- solving the steady part alone is too hard (it is not known how to do that... more later!)

$$\frac{dF(U)}{dr} = S(U)$$

- engineers developed time-marching methods to steady state

hdesterck@uwaterloo.ca

Numerical method

- hyperbolic conservation law

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial r} = S(U)$$

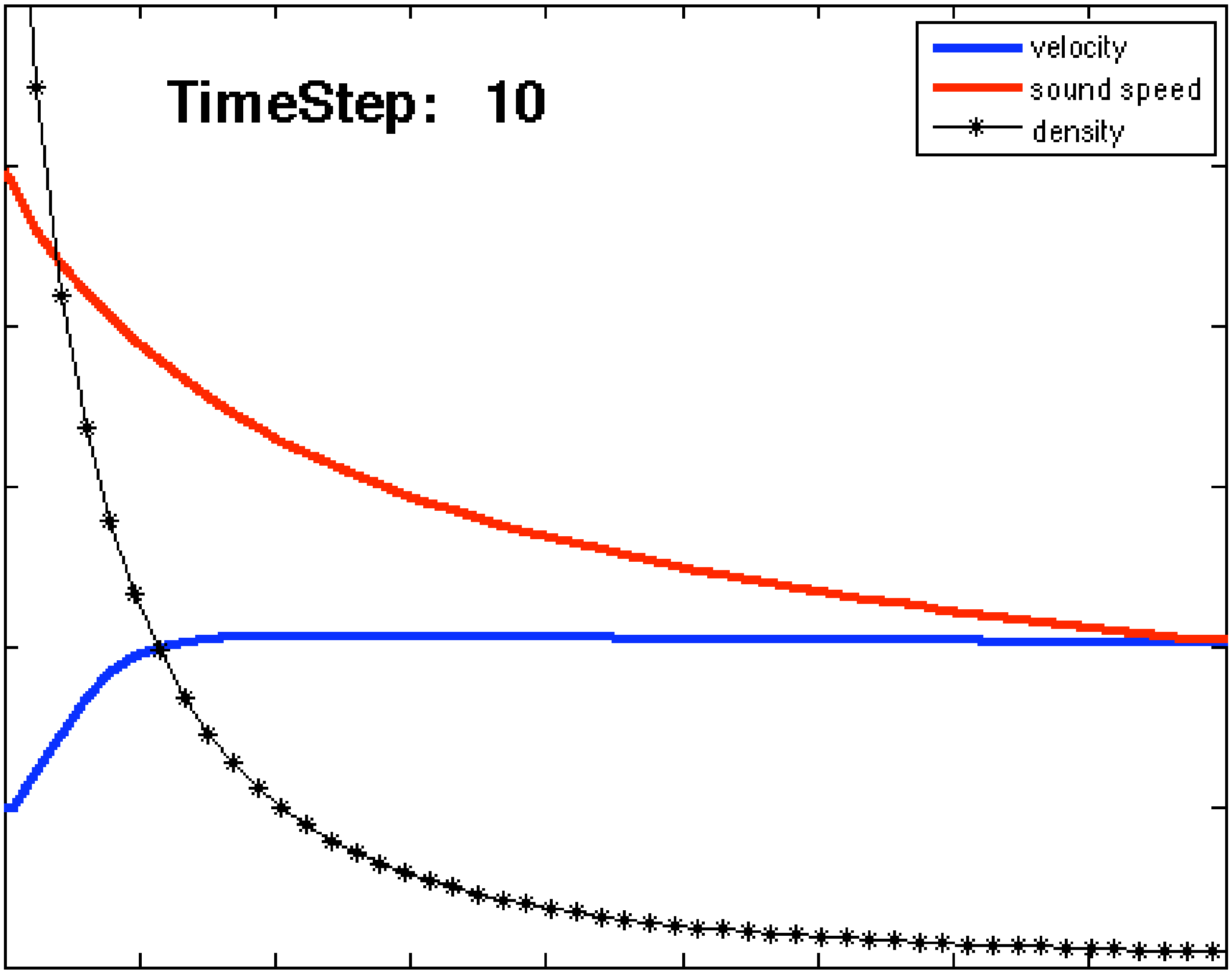
- use Computational Fluid Dynamics methods: finite volume method

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{F^*_{i+1/2} - F^*_{i-1/2}}{\Delta r} = S(U_i)$$

- very slow convergence to steady state... (more later!)

CPA, July 2007
hdesterck@uwaterloo.ca

Simulations of planet atmosphere



University of Waterloo

Results for 1D exoplanet simulations

- HD209458b:
  - lower boundary conditions $\rho=7.10^{-9}$ g/cm^{-3} and T=750K
  - extent of atmosphere, outflow velocity, and mass flux consistent with observations (Vidal-Madjar 2003)
  - 1% mass loss in 12 billion years $\Rightarrow$ HD209458b is stable
- Tian, Toon, Pavlov, and De Sterck, Astrophysical Journal 621, 1049-1060, 2005

CPA, July 2007
hdesterck@uwaterloo.ca

3. Time marching versus solving the unsteady equations directly

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0 \qquad \nabla \cdot \vec{F}(U) = 0$$

- time marching converges slowly
- implicit time integration may help somewhat

$$\frac{U^{n+1} - U^{n}}{\Delta t} + \nabla \cdot \vec{F}(U^{n+1}) = 0$$

- Newton: linearize $\vec{F}$
- Krylov: iterative solution of linear system in every Newton step

CPA, July 2007
hdesterck@uwaterloo.ca

Main advantages of Newton-Krylov approach

- time-marching uses the hyperbolic BCs for steady problem
- ‘physical’ way to find suitable initial conditions for the Newton method in every timestep
- it works! (in the sense that it allows one to converge to a solution, in many cases, with some trial-and-error)

CPA, July 2007
hdesterck@uwaterloo.ca

Disadvantages of Newton-Krylov approach

- number of Newton iterations required for convergence grows as a function of resolution
- number of Krylov iterations required for convergence of the linear system in each Newton step grows as a function of resolution
- grid sequencing/nested iteration: often does not work as well as it could (need many Newton iterations on each level)
- robustness, hard to find general strategy to increase timestep

$\Rightarrow$ Newton-Krylov methodology not very scalable, not very robust, and expensive

CPA, July 2007
hdesterck@uwaterloo.ca

Why not solve the steady equations directly?

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0 \qquad \nabla \cdot \vec{F}(U) = 0$$

- too hard!
- let's try anyway:
  - maybe we can understand why it is difficult
  - maybe we can find a method that is more efficient than implicit time marching
- start in 1D

hdesterck@uwaterloo.ca

4. Solving the steady equations directly

- Simplified 1D problem: radial isothermal Euler

- 2 equations (ODEs), 2 unknowns ($u, \ \rho$)

$$\frac{d}{dr}(\rho u r^2) = 0$$

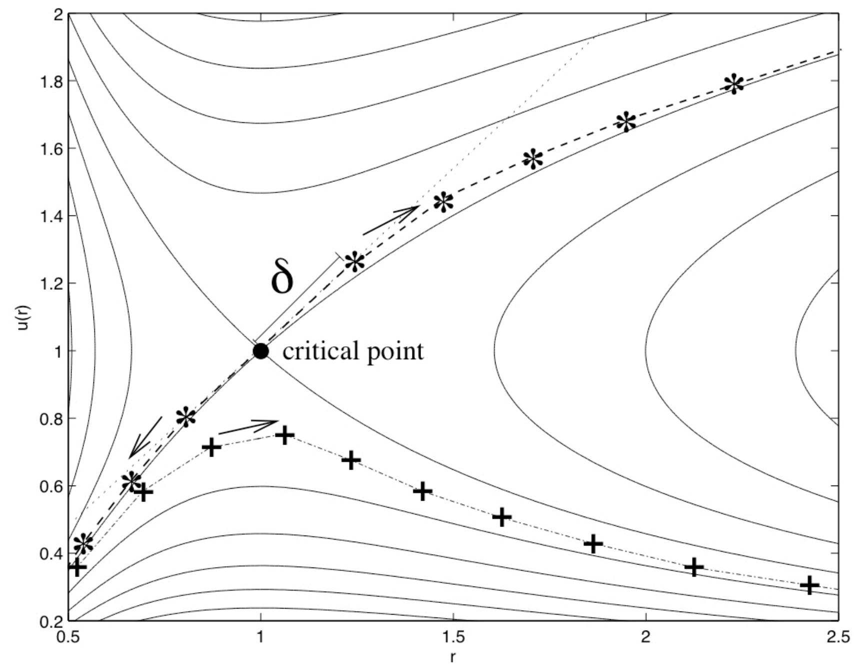
$$\frac{du}{dr} = \frac{2\,u\,c^2\,(r - r_c)}{r^2\,(u^2 - c^2)}$$

University of Waterloo

hdesterck@uwaterloo.ca

Isothermal Euler: solving the steady ODE system is hard...

- solving ODE from the left does not work...
- but... integrating outward from the critical point does work!!!
- also: 2 equations, 2 unknowns, but only 1 BC needed! (along with transonic solution requirement)



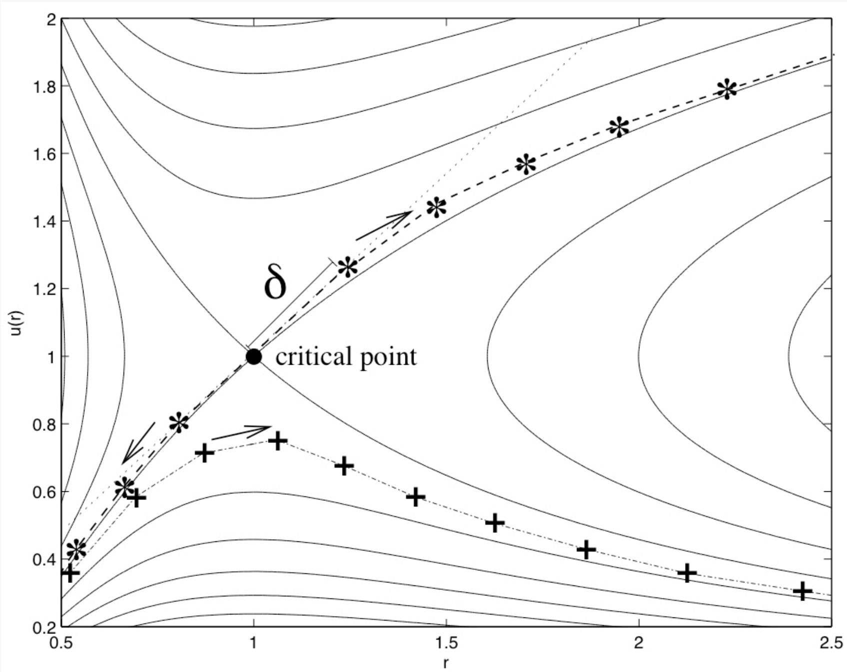
$$\frac{d}{dr}(\rho u r^2) = 0$$

$$\frac{du}{dr} = \frac{2\,u\,c^2\,(r-r_c)}{r^2\,(u^2-c^2)}$$

CPA, July 2007
hdesterck@uwaterloo.ca

Newton Critical Point (NCP) method for steady transonic Euler flows

- First component of NCP: integrate outward from critical point, using dynamical systems formulation



$$\frac{du}{dr} = \frac{2\,u\,c^2\,(r - r_c)}{r^2\,(u^2 - c^2)}$$

University of Waterloo

hdesterck@uwaterloo.ca

First component of NCP

$$\frac{du}{dr} = \frac{2\,u\,c^2\,(r-r_c)}{r^2\,(u^2-c^2)}$$

1. Write as dynamical system...

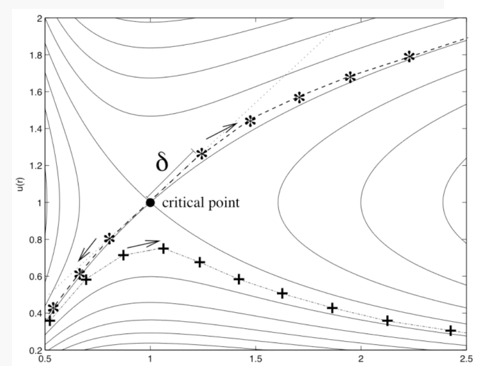
$$\frac{du(s)}{ds} = -2\,u\,c^2\left(r - \frac{GM}{2c^2}\right)$$
$$\frac{dr(s)}{ds} = -r^2\,(u^2 - c^2)$$

$$\frac{dV}{ds} = G(V)$$

2. find critical point: $G(V) = 0$
3. linearize about critical point

$$\left.\frac{\partial G}{\partial V}\right|_{V_{crit}} = \begin{bmatrix} 0 & 2\,c^3 \\ \frac{(GM)^2}{2\,c^3} & 0 \end{bmatrix}$$

4. integrate outward from critical point



For the Full Euler Equations

$$\frac{d}{dr}\begin{bmatrix} \rho\, u\, r^2 \\ \rho\, u^2\, r^2 + p\, r^2 \\ (\frac{\gamma\, p}{\gamma-1} + \frac{\rho\, u^2}{2})\, u\, r^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\rho G M + 2\, p\, r \\ -\rho G M\, u + q_{heat}\, r^2 \end{bmatrix}$$

- 3 equations, 3 unknowns, but only 2 inflow BC
- problem: there are many possible critical points! (two-parameter family)

CPA, July 2007
hdesterck@uwaterloo.ca

Full Euler dynamical system

$$\frac{dF}{ds} = 0,$$

$$\frac{du}{ds} = 2\,u\,c^2\,(r - \frac{GM}{2c^2}) - (\gamma - 1)\,q_{heat}\frac{r^4\,u}{F},$$

$$\frac{dr}{ds} = r^2\,(u^2 - c^2),$$

$$\frac{dT}{ds} = (\gamma - 1)\,T\,(GM - 2\,u^2\,r) - (\gamma - 1)\,q_{heat}\frac{r^4}{F}\,(T - u^2).$$

$$\Longrightarrow \quad T_{crit} = \frac{GM}{2\,\gamma\,r_{crit}} + (\gamma - 1)\,\frac{q_{heat}\,r_{crit}^3}{2\,\gamma\,F_{crit}},$$

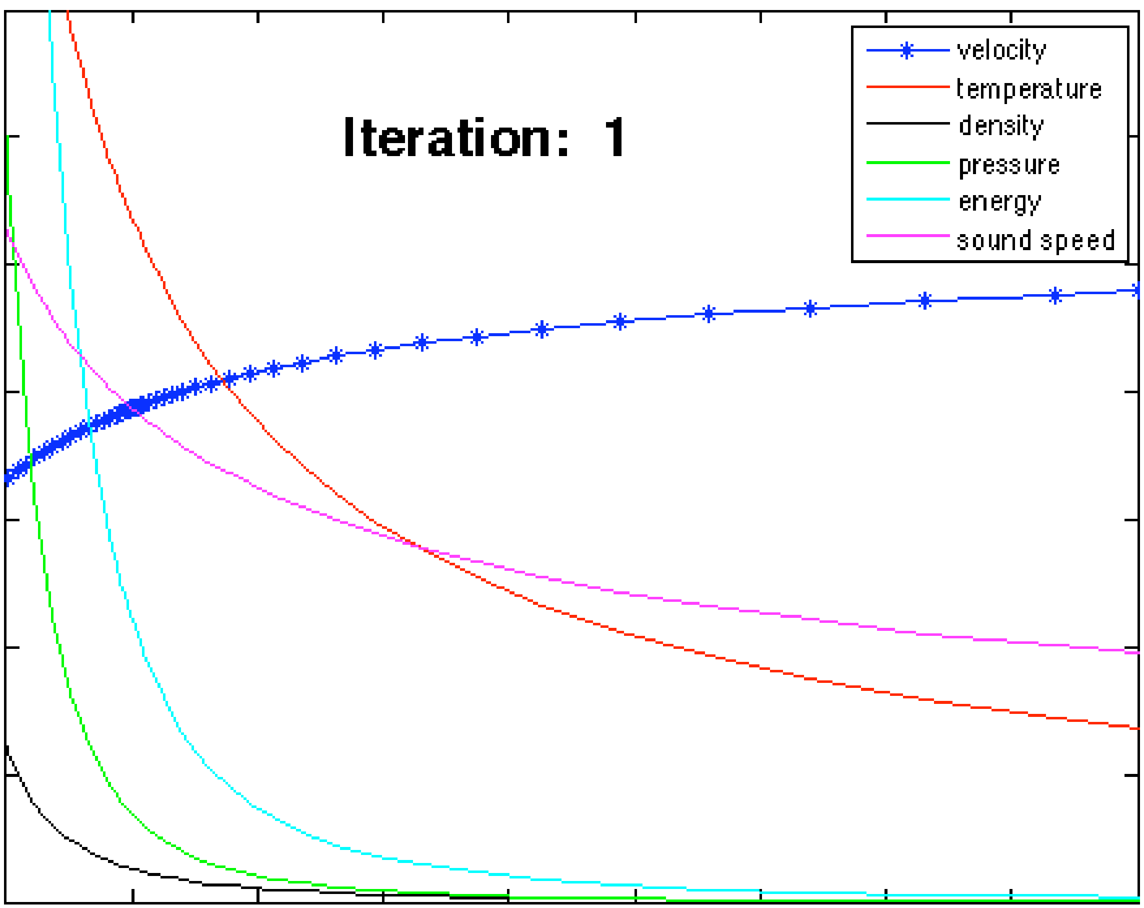
$$u_{crit} = \sqrt{\gamma\,T_{crit}}.$$

CPA, July 2007
hdesterck@uwaterloo.ca

Second component of NCP: use Newton method to match critical point with BCs

guess initial critical point

1. use adaptive ODE integrator to find trajectory
2. modify guess for critical point depending on deviation from desired inflow boundary conditions (2x2 Newton method)
3. repeat



Quadratic Newton covergence

Newton step k	error $\|B^{(k)} - B^*\|_2$
1	4.41106268600662
2	2.28831581534917
3	1.43924405447424
4	0.10259052732943
5	0.00125578478131
6	0.00000037420499

University of Waterloo

CPA, July 2007
hdesterck@uwaterloo.ca

NCP method for 1D steady flows

- it is possible to solve steady equations directly, if one uses critical point and dynamical systems knowledge

- (Newton) iteration is still needed

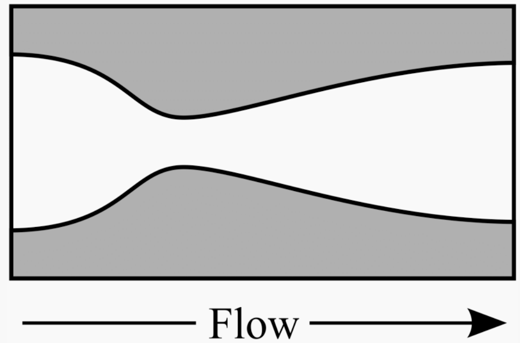
- NCP Newton method solves a 2x2 nonlinear system

(adaptive integration of trajectories is explicit)

- much more efficient than solving a 1500x1500 nonlinear system, and more well-posed

5. Extension to problems with shocks

- consider quasi-1D nozzle flow



$$\frac{\partial}{\partial t}\begin{bmatrix} \rho A \\ \rho u A \\ \left(\frac{p}{\gamma-1}+\frac{\rho u^2}{2}\right) A \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} \rho u A \\ \rho u^2 A + p A \\ \left(\frac{\gamma p}{\gamma-1}+\frac{\rho u^2}{2}\right) u A \end{bmatrix} = \begin{bmatrix} 0 \\ p \frac{dA}{dx} \\ 0 \end{bmatrix}.$$

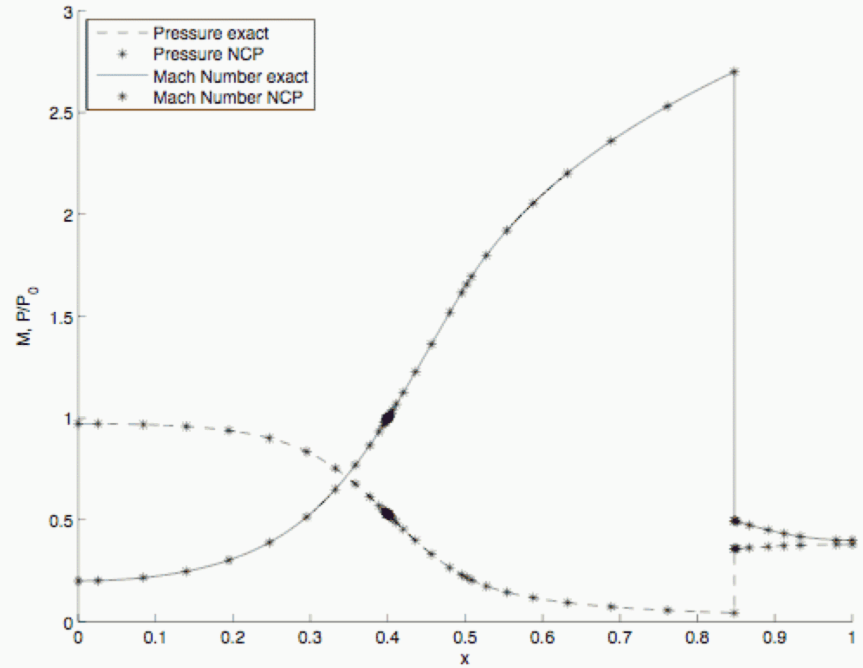
$$\Longrightarrow \quad \begin{aligned} u_{crit} &= \sqrt{\gamma T_{crit}} = c_{crit}, \\ \frac{dA}{dx}(x_{crit}) &= 0. \end{aligned}$$

NCP method for nozzle flow with shock

- subsonic in: 2 BC
- subsonic out: 1 BC

- NCP from critical point to match 2 inflow BC

- Newton method to match shock location to outflow BC (using Rankine-Hugoniot relations, 1 free parameter)



6. Extension to problems with heat conduction

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho\, r^2 \\ \rho\, u\, r^2 \\ \left(\frac{p}{\gamma-1}+\frac{\rho\, u^2}{2}\right)\, r^2 \end{bmatrix} + \frac{\partial}{\partial r}\begin{bmatrix} \rho\, u\, r^2 \\ \rho\, u^2\, r^2 + p\, r^2 \\ \left(\frac{\gamma\, p}{\gamma-1}+\frac{\rho\, u^2}{2}\right)\, u\, r^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\rho\, G M + 2\, p\, r \\ -\rho\, G M\, u + q_{heat}\, r^2 + \frac{\partial}{\partial r}\left(\kappa\, r^2\, \frac{\partial T}{\partial r}\right) \end{bmatrix}$$

University of Waterloo

Dynamical system for Euler with heat conduction

$$\phi = \kappa\, r^2 \tfrac{dT}{dr}$$

$$\begin{aligned}
\frac{dr}{ds} &= -r^2(u^2-c^2)(u^2-T),\\
\frac{dF}{ds} &= 0,\\
\frac{du}{ds} &= -2uc^2\left(r-\frac{GM}{2c^2}\right)(u^2-T)+\frac{\phi u(u^2-c^2)}{\kappa}\\
&\quad -(\gamma-1)uT(GM-2u^2r),\\
\frac{dT}{ds} &= \frac{-\phi(u^2-c^2)(u^2-T)}{\kappa},\\
\frac{d\phi}{ds} &= \frac{-\phi F(u^2-c^2)^2}{(\gamma-1)\kappa}+FT(GM-2u^2r)(u^2-c^2)\\
&\quad +q_{heat}r^4(u^2-c^2)(u^2-T).
\end{aligned}$$

CPA, July 2007
hdesterck@uwaterloo.ca

Two types of critical points!

- sonic critical point (node):

$$u_{crit} = \sqrt{\gamma T_{crit}} = c_{crit}$$

- thermal critical point (saddle point):

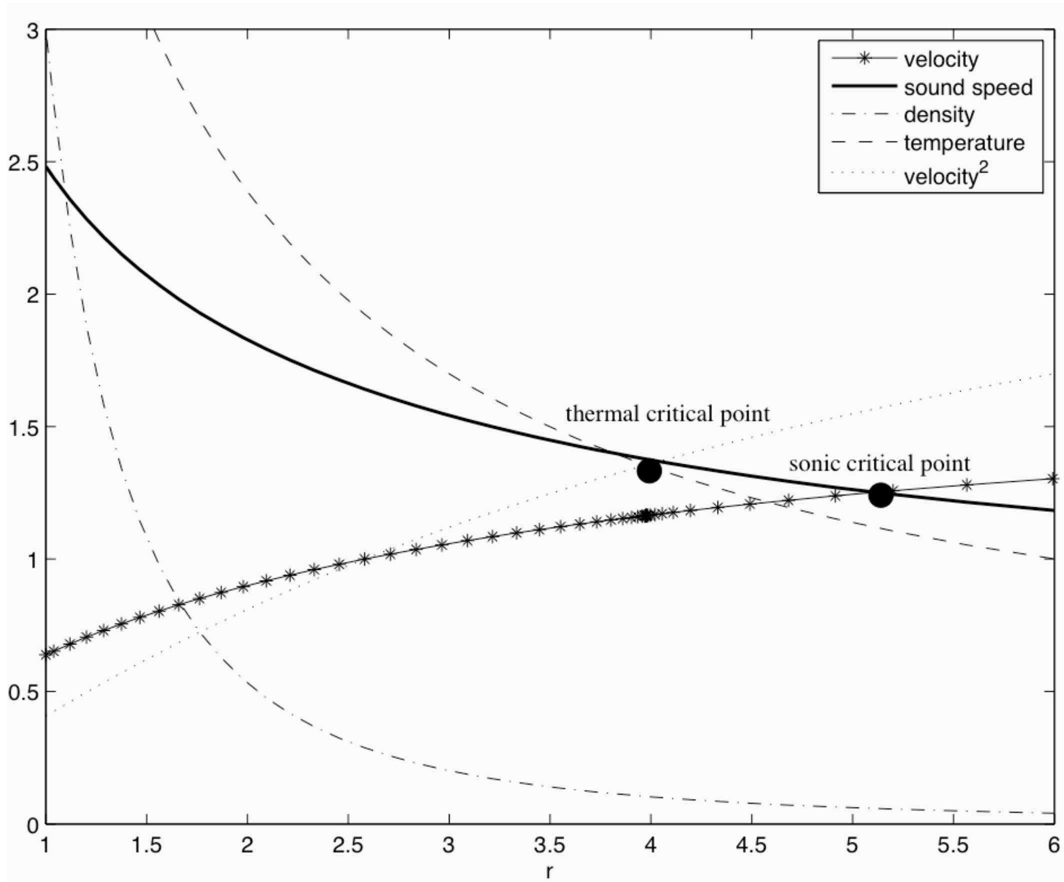
$$\begin{aligned} u_{crit} &= \sqrt{T_{crit}} = c_{crit}/\sqrt{\gamma}, \\ \frac{\phi_{crit}}{\kappa} + GM - 2u_{crit}^2 r_{crit} &= 0. \end{aligned}$$

University of Waterloo

hdesterck@uwaterloo.ca

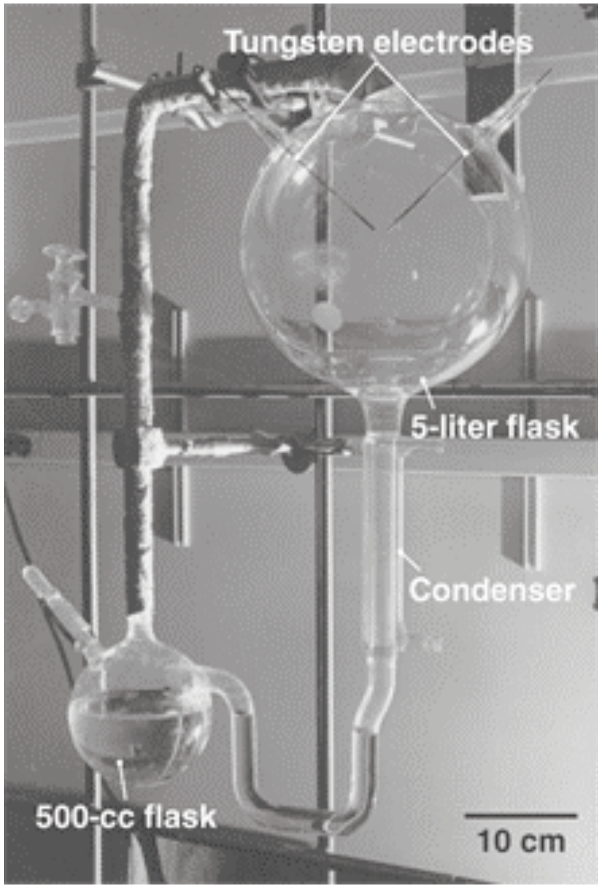
Transonic flow with heat conduction

- subsonic inflow: 3 BC (ρ, p, φ)
- supersonic outflow: 0 BC
- 3-parameter family of thermal critical points
- NCP matches thermal critical point with 3 inflow BC
- SIAM Journal on Applied Dynamical Systems, to appear



University of Waterloo

7. Second application: primordial soup as the origin of life on Earth



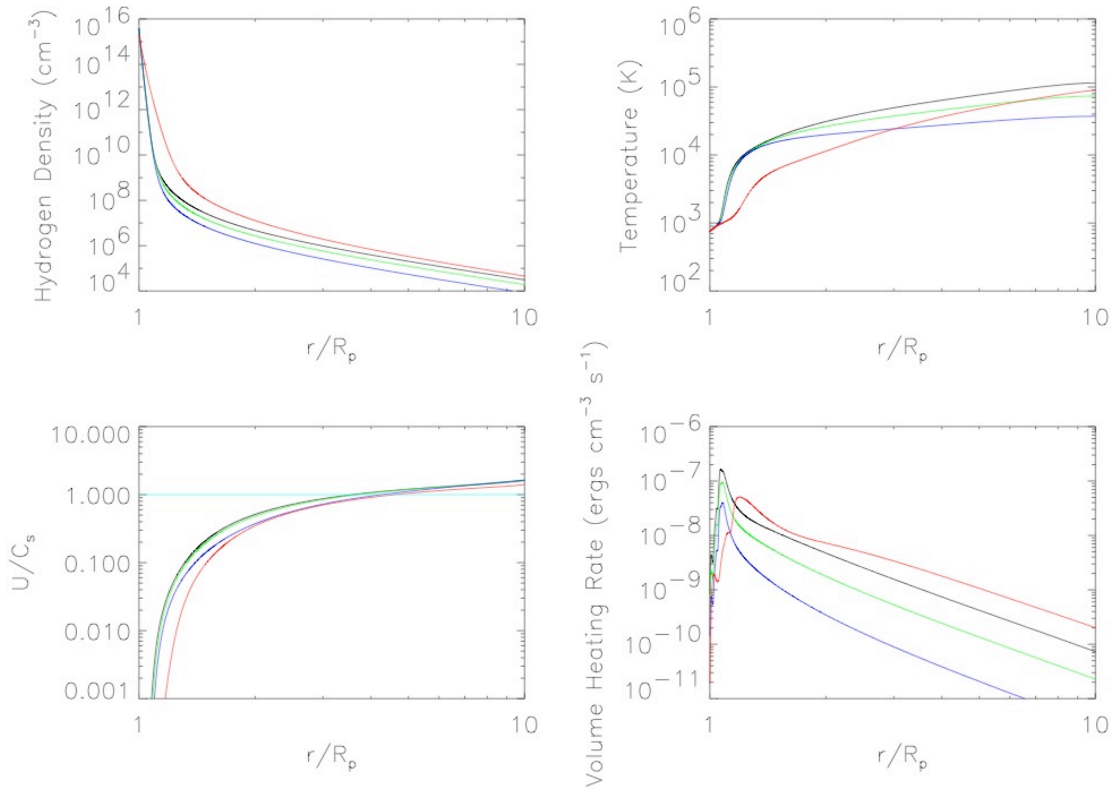
- Stanley Miller (1953): formation of prebiotic molecules in a CH4-NH3 rich environment with electric discharge
  - -Problem: CH4-NH3 atmosphere unlikely
- later experiments show that prebiotic molecules can be formed efficiently in a hydrogen-rich environment
- alternative sources of organics: hydrothermal system, comet delivery

hydrogen content in Early Earth atmosphere

- hydrogen content: balance between volcanic outgassing and escape from atmosphere
- existing theory: static atmosphere with high temperature at top $\Rightarrow$ fast thermal escape $\Rightarrow$ hydrogen content was very low
- formation of prebiotic molecules in a hydrogen-rich atmosphere was thus discarded as a theory

new theory: hydrogen content in Early Earth atmosphere

- our results: hydrogen escape was probably supersonic, with low temperature at top (no thermal escape), and total escape rates were low



University of Waterloo

CPA, July 2007
hdesterck@uwaterloo.ca

hydrogen content in Early Earth atmosphere

- our results: hydrogen concentration in the atmosphere of Early Earth could have been as high as 30%
- formation of prebiotic molecules in early Earth's atmosphere could have been efficient $\Rightarrow$ primordial soup on early Earth is possible
- no need for hydrothermal vents, cometary delivery
- Tian, Toon, Pavlov, and De Sterck, Science 308, 1014-1017, 2005

8. Conclusions

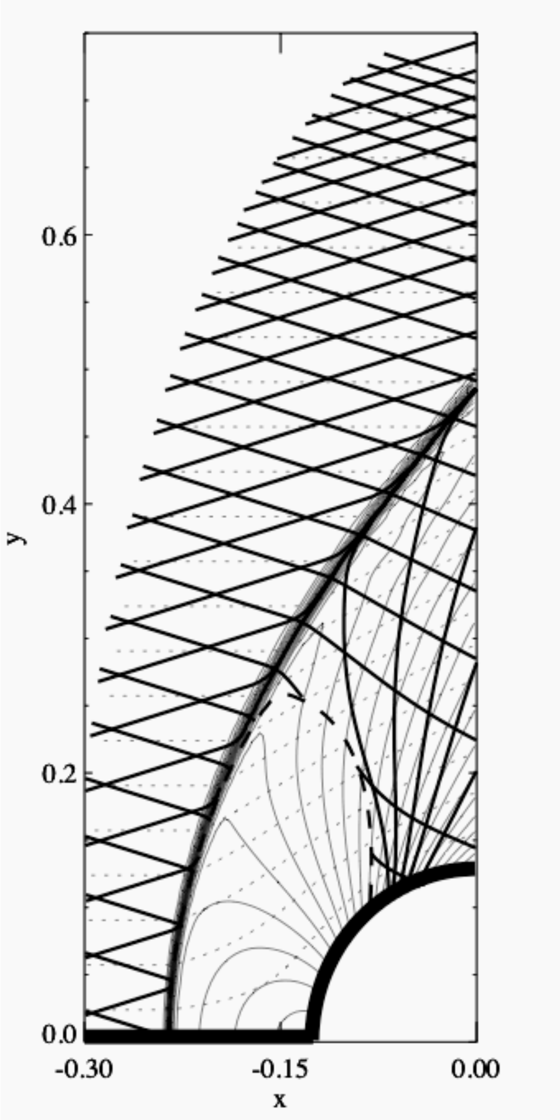
- 1D models of supersonic hydrogen escape from planetary atmospheres developed (exoplanets and early Earth)
- solving steady Euler equations directly is superior to time-marching methods for 1D transonic flows
- Newton Critical Point (NCP) uses
  - adaptive itegration outward from critical point
  - dynamical system formulation
  - 2x2 Newton method to match critical point with BC

Conclusions

- 2D NCP: work in progress

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0$$

$$\nabla \cdot \vec{F}(U) = 0$$



University of Waterloo

Conclusions

- 2D: work in progress
  - integrate separately in different domains of the flow, 'outward' from critical curves (shocks and limiting lines)
  - match conditions at critical curves with BCs using Newton method
  - issues:
    - change of topology
    - solve PDE in different regions
    - cost
  - potential advantages are significant: problem more well-posed
    - separate nonlinear singularities from smooth flow calculations
    - fixed number of Newton steps, linear iterations (scalable)
    - better grid sequencing (nested iteration)

hdesterck@uwaterloo.ca