Efficient Numerical Simulation of ODE and PDE Fluid Flow Solutions with Critical Points and Shocks

Hans De Sterck

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

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Differential and Differential-Algebraic Equations
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this presentation is about ...

- applications in computational fluid dynamics - stationary compressible fluid flows
- flow solutions with elliptic (subsonic) and hyperbolic (supersonic) regions separated by critical points and shocks
- how to calculate such flow solutions efficiently
- not the traditional time-marching methods
- PDEs (multi-D) and ODEs (1D)
- some elements of dynamical systems

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hdesterck@uwaterloo.ca

1. Motivation and context

- consider stationary solutions of hyperbolic conservation law (PDE)

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

- in particular, compressible Euler equations

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho\,\vec{v} \\ \frac{p}{\gamma-1} + \frac{\rho\,v^2}{2} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho\,\vec{v} \\ \rho\,\vec{v}\vec{v} + I\,p \\ (\frac{\gamma\,p}{\gamma-1} + \frac{\rho\,v^2}{2})\,\vec{v} \end{bmatrix} = 0$$

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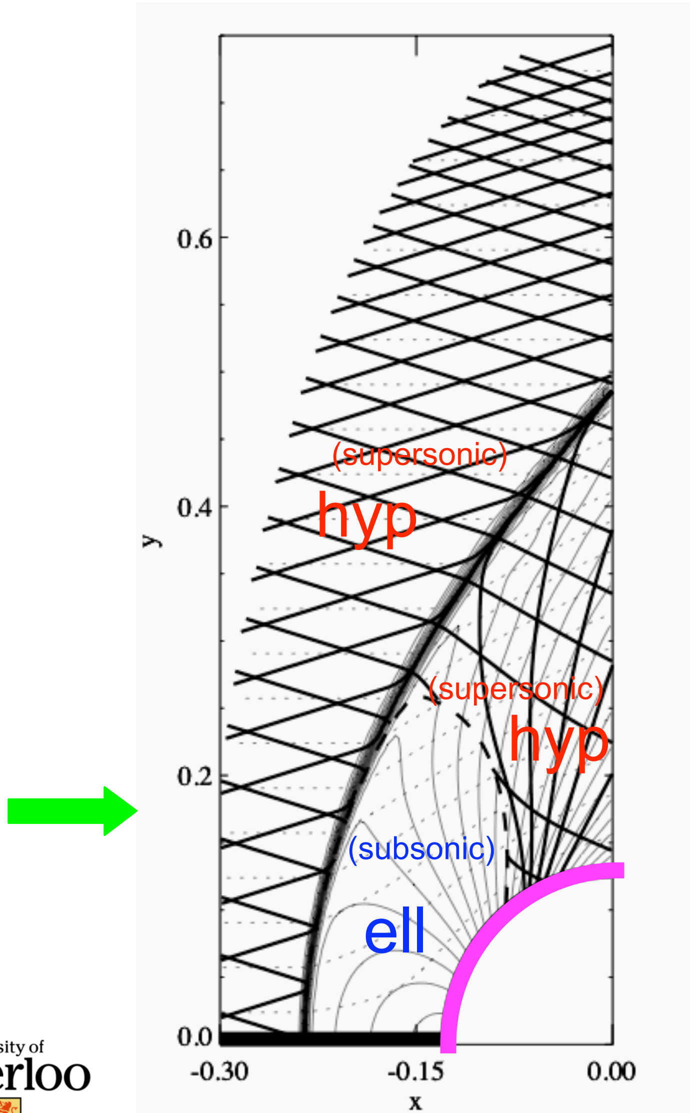
Transonic steady Euler flows



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

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

$$\nabla \cdot \begin{bmatrix} \rho\, \vec{v} \\ \rho\, \vec{v}\vec{v} + I\, p \\ (\frac{\gamma\, p}{\gamma - 1} + \frac{\rho\, v^2}{2})\, \vec{v} \end{bmatrix} = 0$$

Standard approach for steady flow simulation

- time marching (often implicit)

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

- Newton: linearize $\vec{F}$
- Krylov: iterative solution of linear system in every Newton step
- Schwarz: parallel (domain decompositioning), or multigrid

$\Rightarrow$ NKS methodology for steady flows

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Main advantages of NKS

- use 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)

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Disadvantages of NKS

- number of Newton iterations required for convergence can grow as a function of resolution
- number of Krylov iterations required for convergence of the linear system in each Newton step can grow 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

$\Rightarrow$ NKS methodology not very scalable, and expensive

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! (BCs, elliptic-hyperbolic, ...)
- 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 (ODE)

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2. 1D model problems (ODE systems)

- radial outflow from extrasolar planet

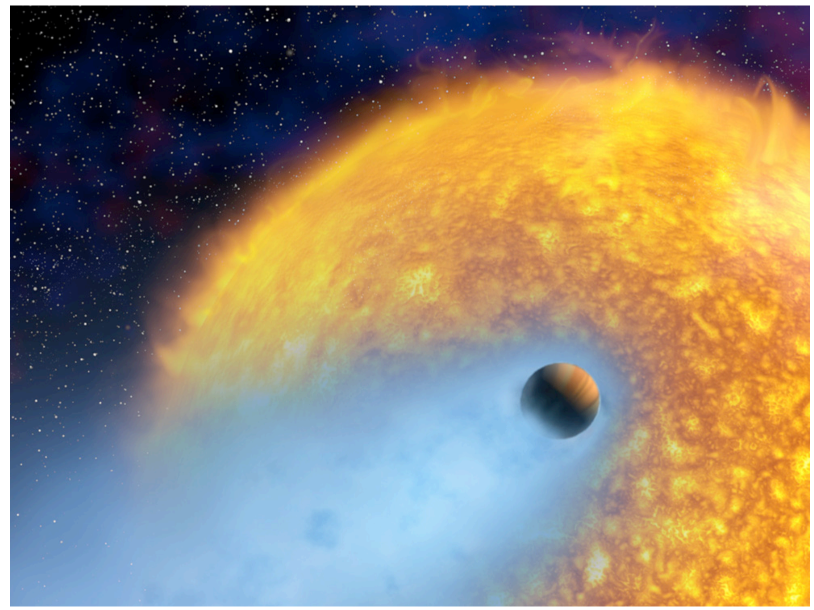
$$\frac{\partial}{\partial t}\begin{bmatrix} \rho\, r^2 \\ \rho\, u\, r^2 \\ (\frac{p}{\gamma-1}+\frac{\rho\, u^2}{2})\, r^2 \end{bmatrix} + \frac{\partial}{\partial r}\begin{bmatrix} \rho\, u\, r^2 \\ \rho\, u^2\, r^2 + p\, r^2 \\ (\frac{\gamma\, p}{\gamma-1}+\frac{\rho\, u^2}{2})\, u\, r^2 \end{bmatrix}$$

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

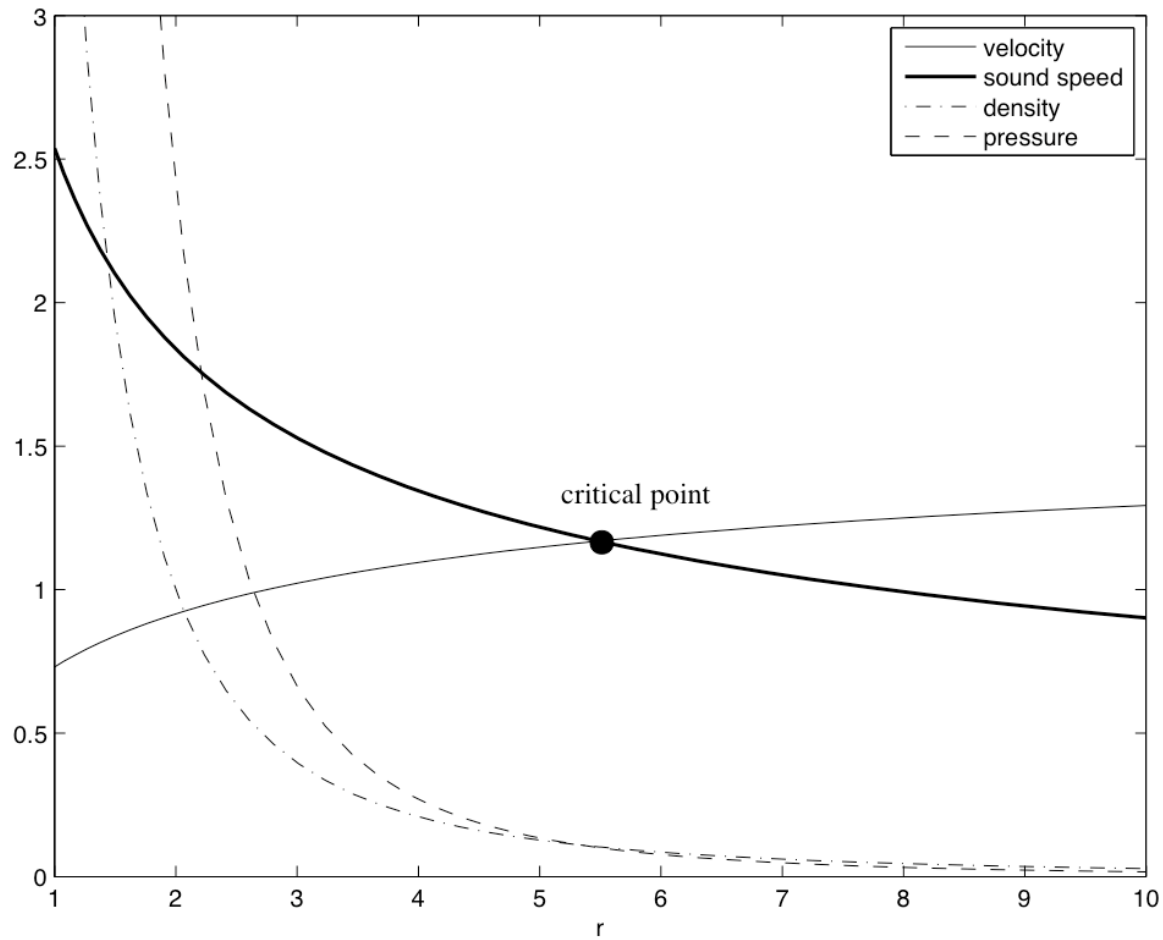
hdesterck@uwaterloo.ca

Radial outflow from exoplanet

- http://exoplanet.eu
- 374 extrasolar planets known, as of September 2009
- 39 multiple planet systems
- many exoplanets are gas giants ("hot Jupiters")
- many orbit very close to star (~0.05 AU)
- hypothesis: strong irradiation leads to supersonic hydrogen escape



Transonic radial outflow solution of Euler equations of gas dynamics



subsonic ⇒|⇐ supersonic

(also: Parker's solar wind, ...)

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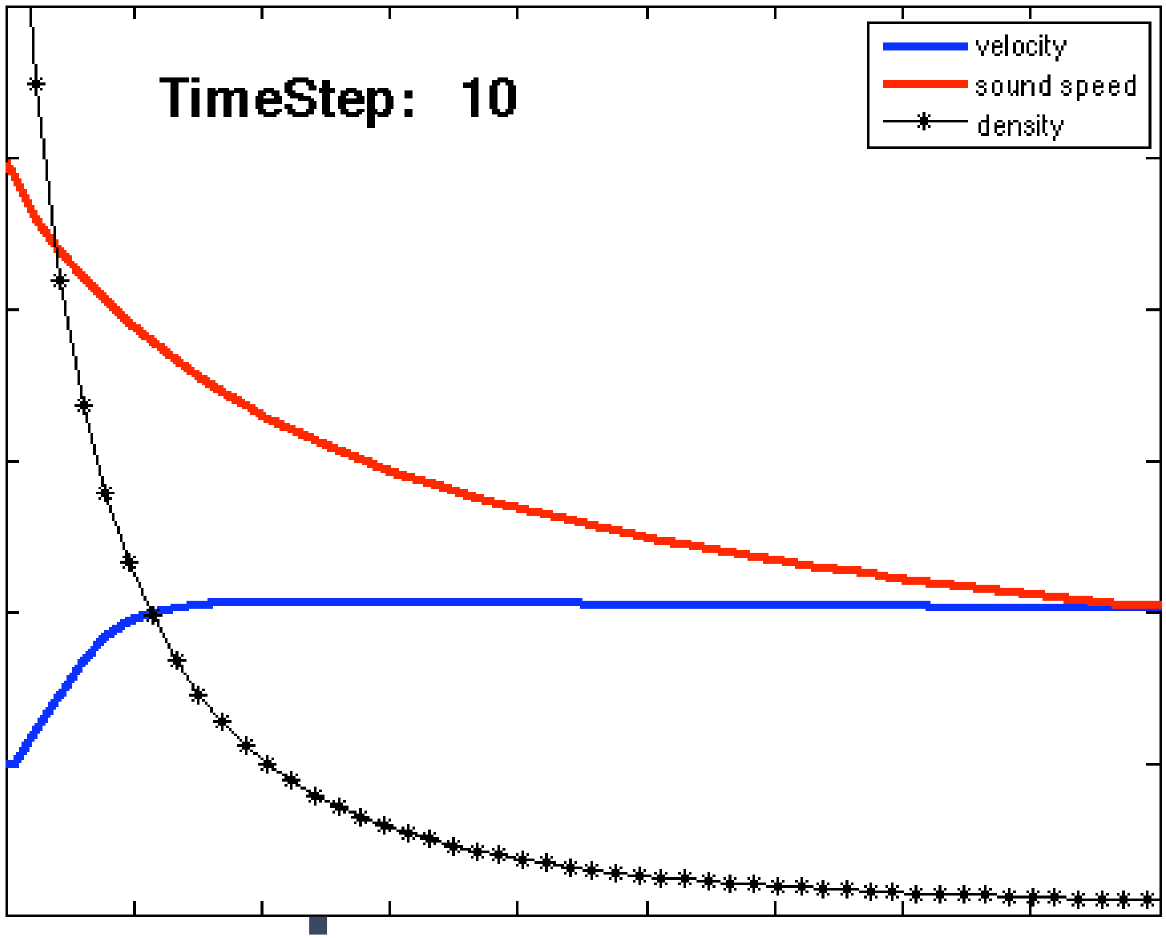
Use time marching method (explicit)



$v - c = 0$

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Simplified 1D problem: radial isothermal Euler

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

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

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

hdesterck@uwaterloo.ca

Solving the steady ODE system is hard...

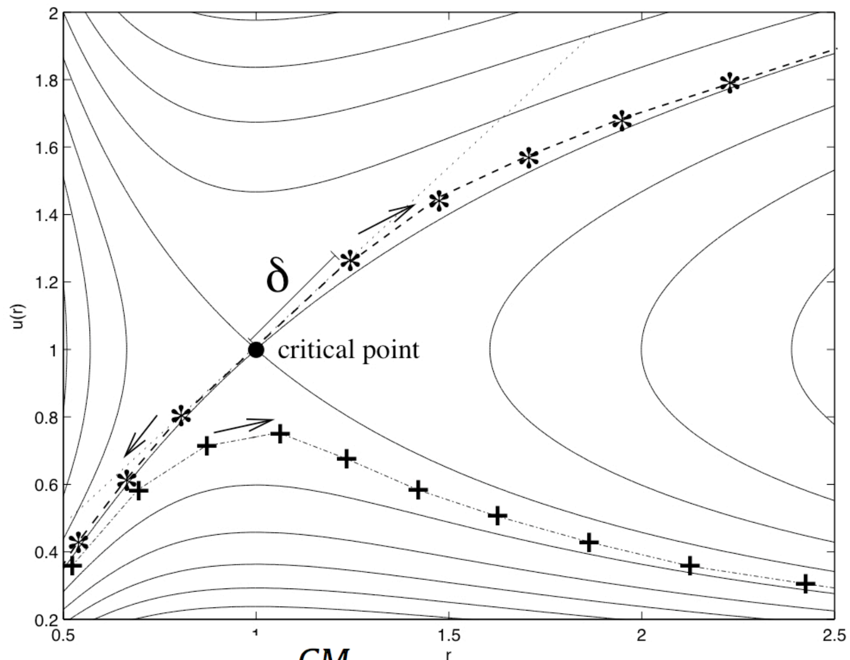
- critical point:

  2 equations, 2 unknowns, but only 1 BC needed: ρ_0 ! (along with transonic solution requirement)

  (no u_0 required!)

- solving ODE from the left does not work...

- but... integrating outward from the critical point does work!!!



ρ_0

no u_0!

$$r_{crit} = \frac{GM}{2c^2}$$

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

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

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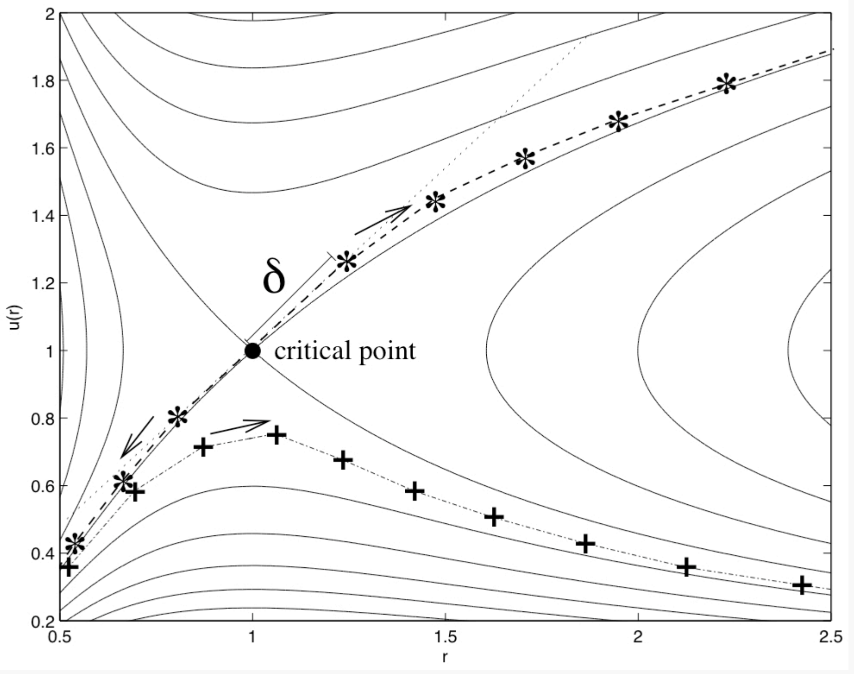
3. Newton Critical Point (NCP) method for ODE steady transonic Euler flows

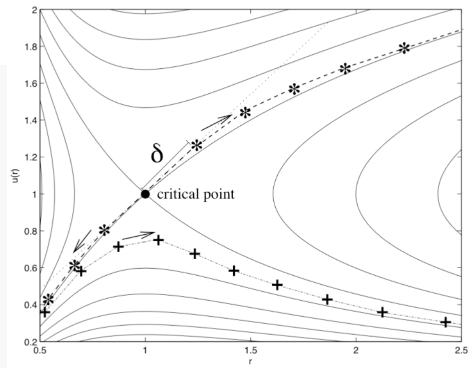
- First component of NCP: integrate outward from critical point, using dynamical systems formulation



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

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, eigenvectors

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

4. integrate outward from critical point

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hdesterck@uwaterloo.ca

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 (ρ_0, p_0) (u_0 results from simulation)
- problem: there are many possible critical points! (two-parameter family)

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Full Euler dynamical system

$$
\begin{aligned}
\frac{dF}{ds} &= 0, \\
\frac{du}{ds} &= 2\,u\,c^2\,(r - \frac{GM}{2c^2}) - (\gamma - 1)\,q_{heat}\frac{r^4\,u}{F}, \\
\frac{dr}{ds} &= r^2\,(u^2 - c^2), \\
\frac{dT}{ds} &= (\gamma - 1)\,T\,(GM - 2\,u^2\,r) - \\
&\quad (\gamma - 1)\,q_{heat}\frac{r^4}{F}\,(T - u^2).
\end{aligned}
$$

$$
\Rightarrow \qquad
\begin{aligned}
T_{crit} &= \frac{GM}{2\,\gamma\,r_{crit}} + (\gamma - 1)\,\frac{q_{heat}\,r_{crit}^3}{2\,\gamma\,F_{crit}}, \\
u_{crit} &= \sqrt{\gamma\,T_{crit}}.
\end{aligned}
$$

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hdesterck@uwaterloo.ca

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

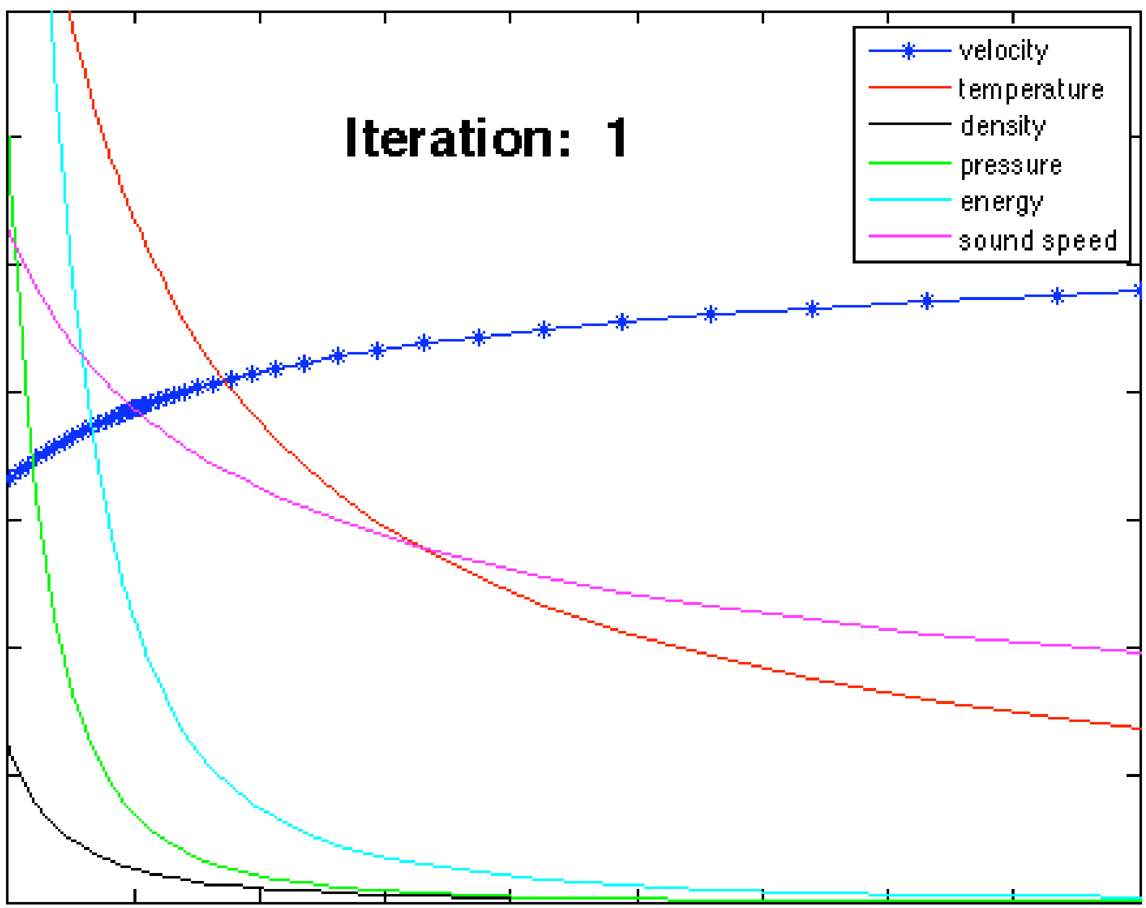
nonlinear shooting method:

guess initial critical point

1. use adaptive ODE integrator to find trajectory (RK45)
2. modify guess for critical point depending on deviation from desired inflow boundary conditions (2x2 Newton method)

   $$\text{find } \mathbf{C} \quad \text{s.t. } \mathbf{B}^* = \mathbf{F}(\mathbf{C})$$

   $$\mathbf{C}^{(\mathbf{k+1})} = \mathbf{C}^{(\mathbf{k})} + \left(J|_{\mathbf{C}^{(\mathbf{k})}}\right)^{-1} \left(\mathbf{B}^* - \mathbf{B}^{(\mathbf{k})}\right)$$
3. repeat



ρ_0

p_0

u_0

hdesterck@uwaterloo.ca

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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

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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

Journal of Computational and Applied Mathematics 223 (2009) 916–928

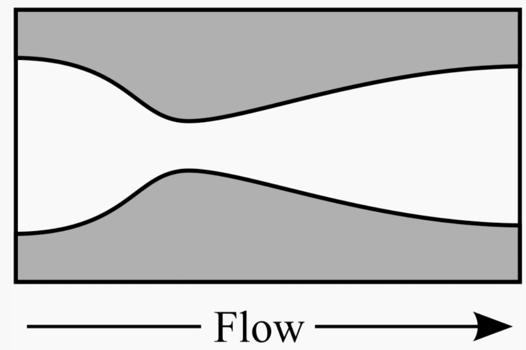
A fast and accurate algorithm for computing radial transonic flows

Hans De Sterck[a,*], Scott Rostrup[a], Feng Tian[b]

hdesterck@uwaterloo.ca

4. Extension to problems with shocks

- consider quasi-1D nozzle flow



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

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

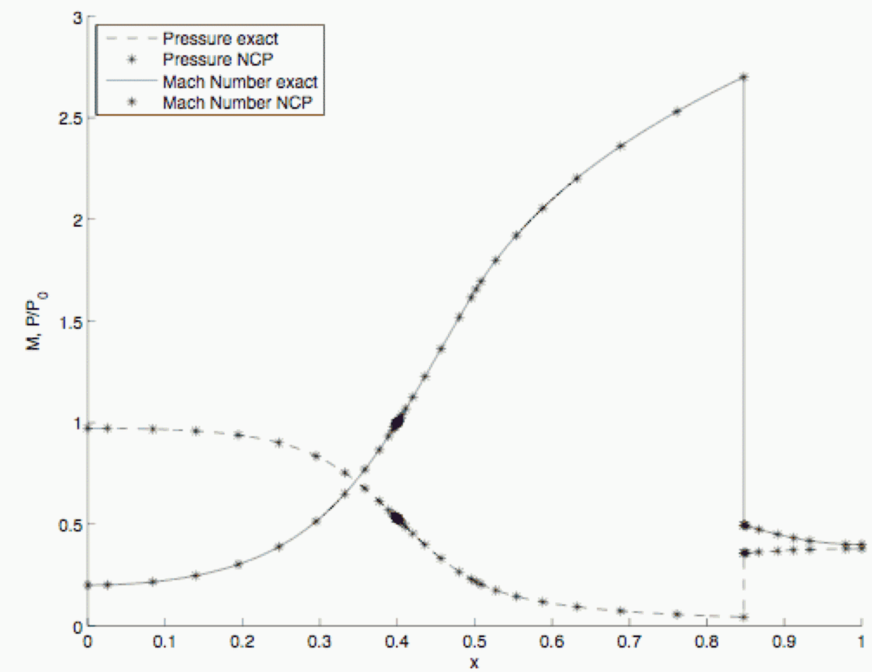
hdesterck@uwaterloo.ca

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)



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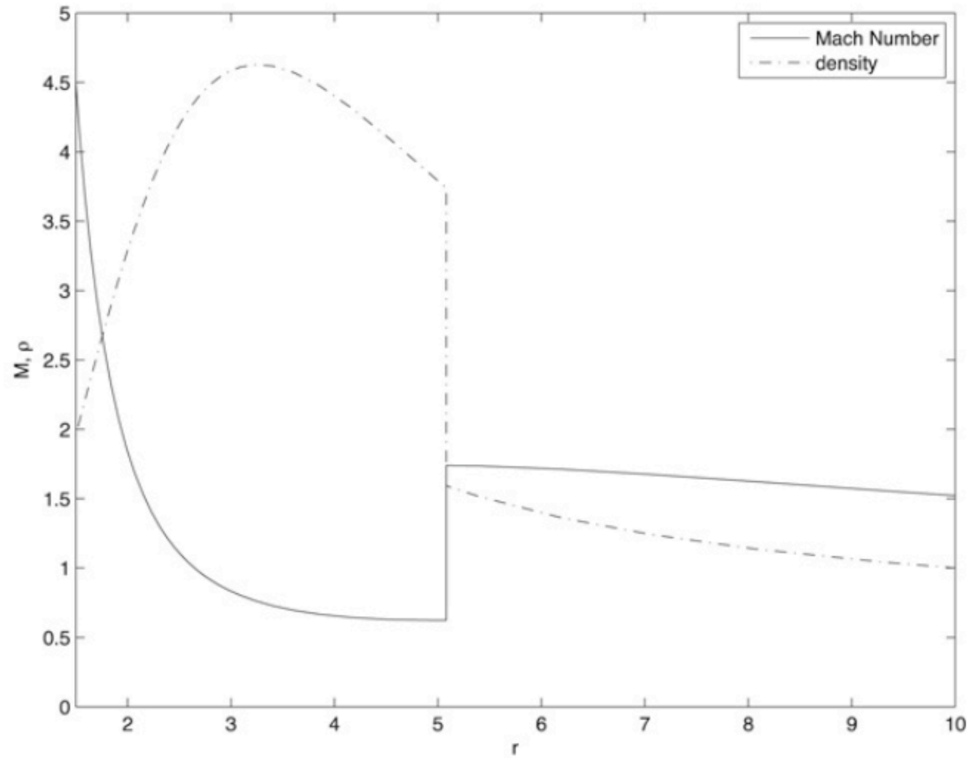
Other application: black hole accretion



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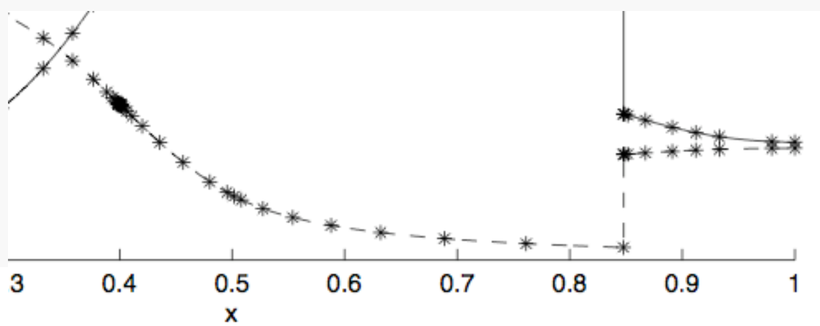
Some thoughts

- positive at shock... (monotone, no oscillations)
- no limiter was required... (=no headache)
- as accurate as you want, with error control (adaptive RK45 in smooth parts, Newton with small tolerance at singularities)
- small Newton systems at singularities (one dimension smaller than problem), low cost, good scaling
- if only we could do something like this in 2D, 3D, time-dependent!



hdesterck@uwaterloo.ca

5. Extension to problems with heat conduction

SIAM J. APPLIED DYNAMICAL SYSTEMS
Vol. 6, No. 3, pp. 645–662

Critical Point Analysis of Transonic Flow Profiles with Heat Conduction*

H. De Sterck†

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

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Dynamical system for Euler with heat conduction

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

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

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hdesterck@uwaterloo.ca

Two critical points of different type!

- sonic critical point (node):

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

- thermal critical point (saddle point):

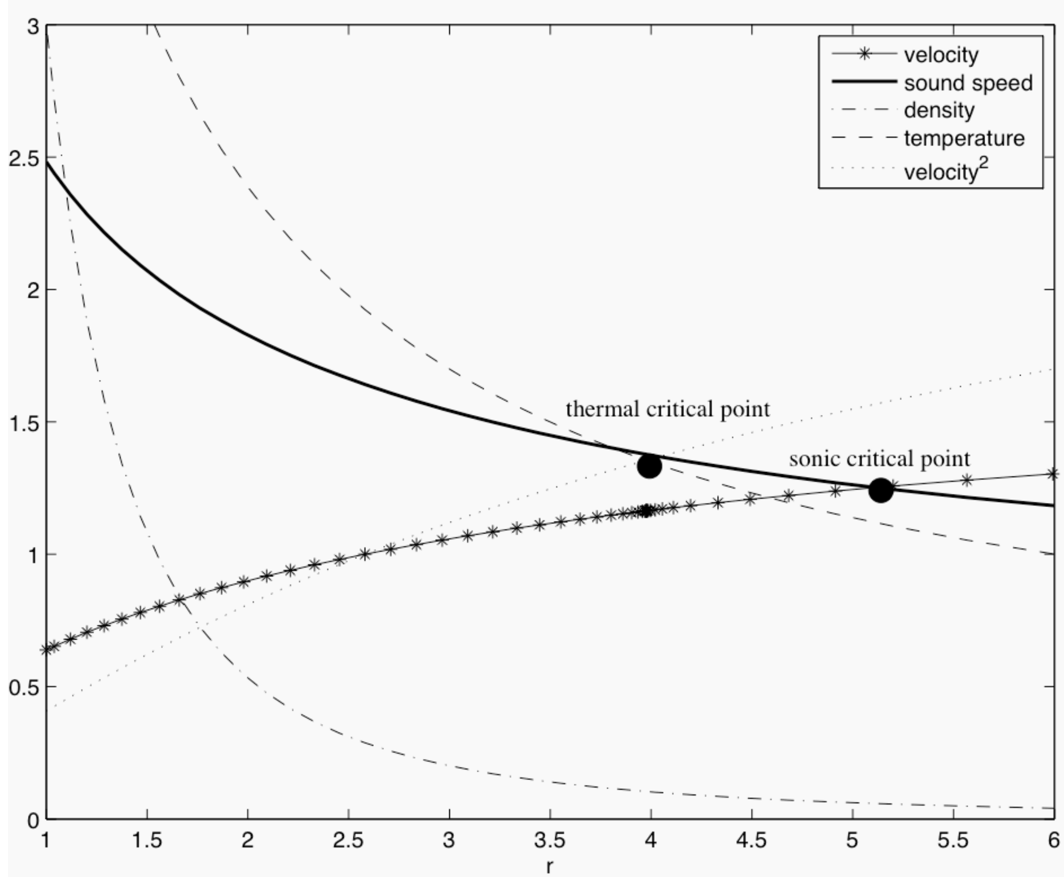
$$\begin{aligned} u_{crit} &= \sqrt{T_{crit}} = c_{crit}/\sqrt{\gamma}, \\ \frac{\phi_{crit}}{\kappa} + GM - 2u_{crit}^2 r_{crit} &= 0. \end{aligned}$$

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

ρ_0
p_0
ϕ_0
u_0



hdesterck@uwaterloo.ca

Further extensions being considered

- viscosity:
  - some preliminary investigation indicates that no new critical points are introduced
  - needs further investigation
- robustness:
  - Newton method can ‘shoot’ to negative density or pressure when approaching inner boundary
  - often, desired solutions lie very close to ‘border’ of feasible/physical parameter domain
  - need a more robust nonlinear system solver (line search, trust region, ...)
- if topology is not known in advance: level sets?

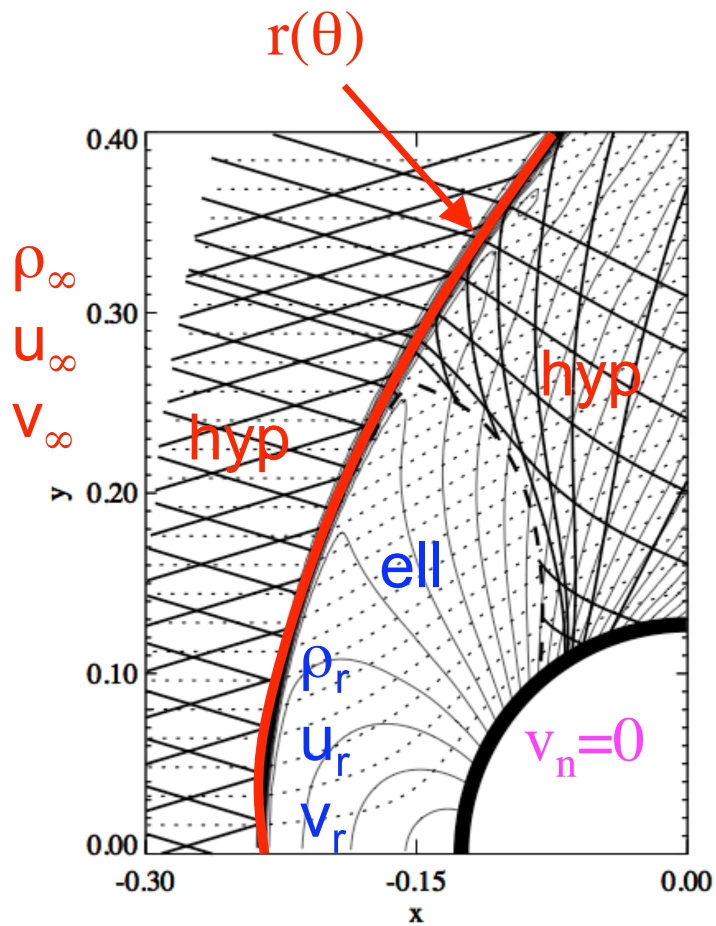
hdesterck@uwaterloo.ca

6. Extension to 2D, 3D: bow shock flows

- assume isothermal flow:

  ρ, u, v
- parametrize shock curve: $r(\theta)$
- discretize: $r_i=r(\theta_i)$
- given ρ_∞, u_∞, v_∞ and $r(\theta)$, use RH relations to get

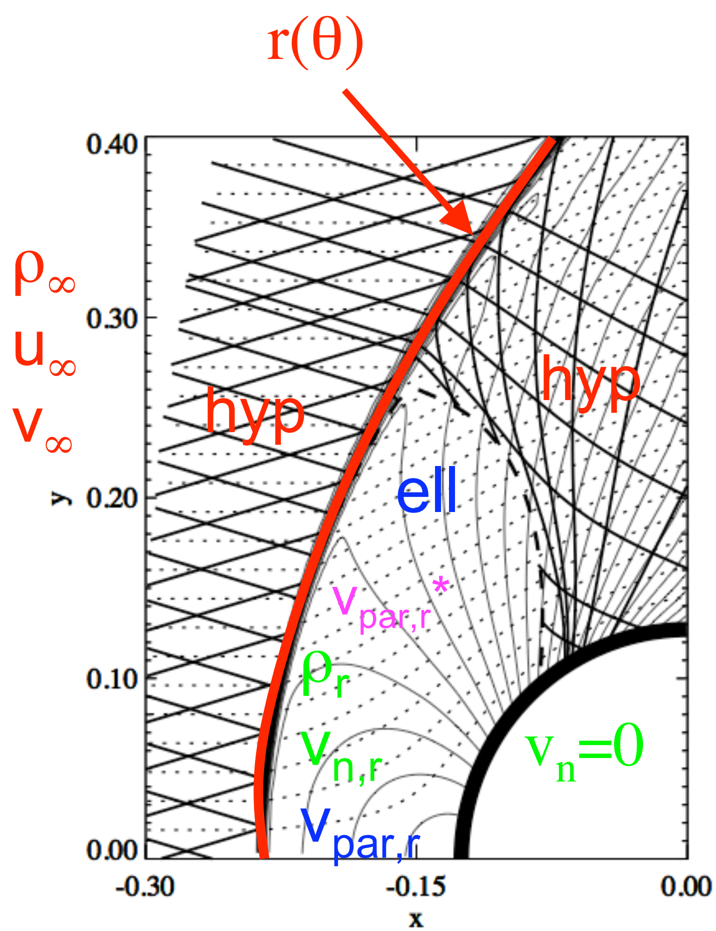
  ρ_r, u_r, v_r
- solve PDE using (nonlinear) FD method in smooth region on right of shock, with BC ρ_r, u_r, v_r
- adjust r_i until $v_n=0$ at wall (1D Newton procedure on $F(r_i)=0$, dense matrix)
- does not work since marching FD is unstable in elliptic region!



hdesterck@uwaterloo.ca

bow shock flows

- solution: solve PDE using (nonlinear) FD method in smooth region on right of shock, with BC ρ_{r}, $v_{n,r}$, $v_{par,r}=0$, this gives $v_{par,r}^*$
- adjust r_i until $v_{par,r}^* = v_{par,r}$ at shock (1D Newton procedure on $F(r_i)=0$, dense matrix)



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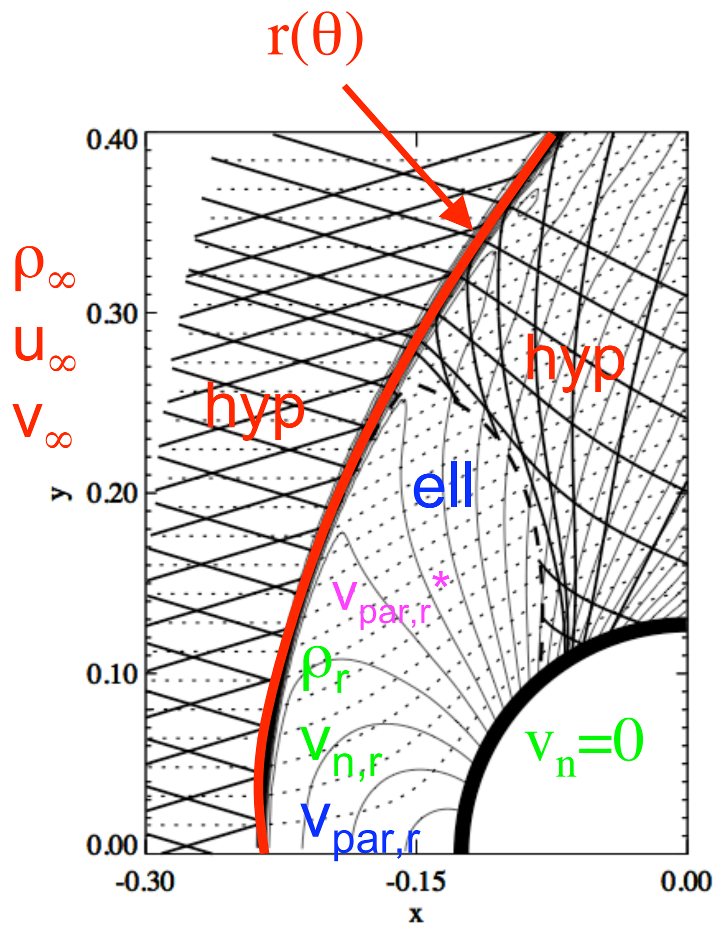
bow shock flows

- we keep from 1D:
  - smaller-size Newton problem (1D instead of 2D)
  - we can use simple high-order FD method for smooth flow region
- worse than in 1D:
  - dense Jacobian
  - need to iterate to solve nonlinear PDE in smooth region
- this may work
- note similarity with shock capturing
- efficiency?; robustness?



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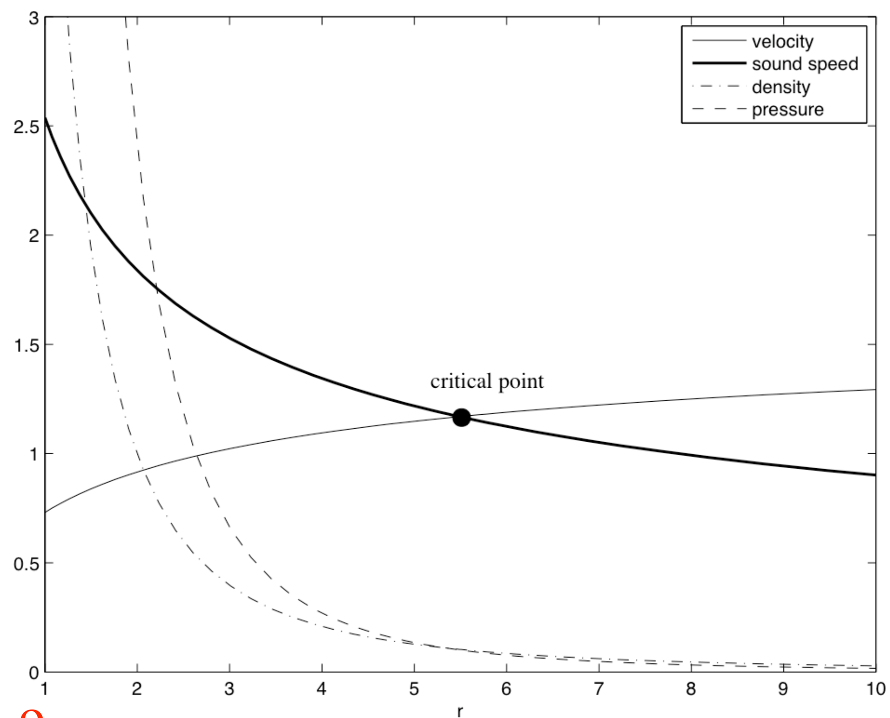
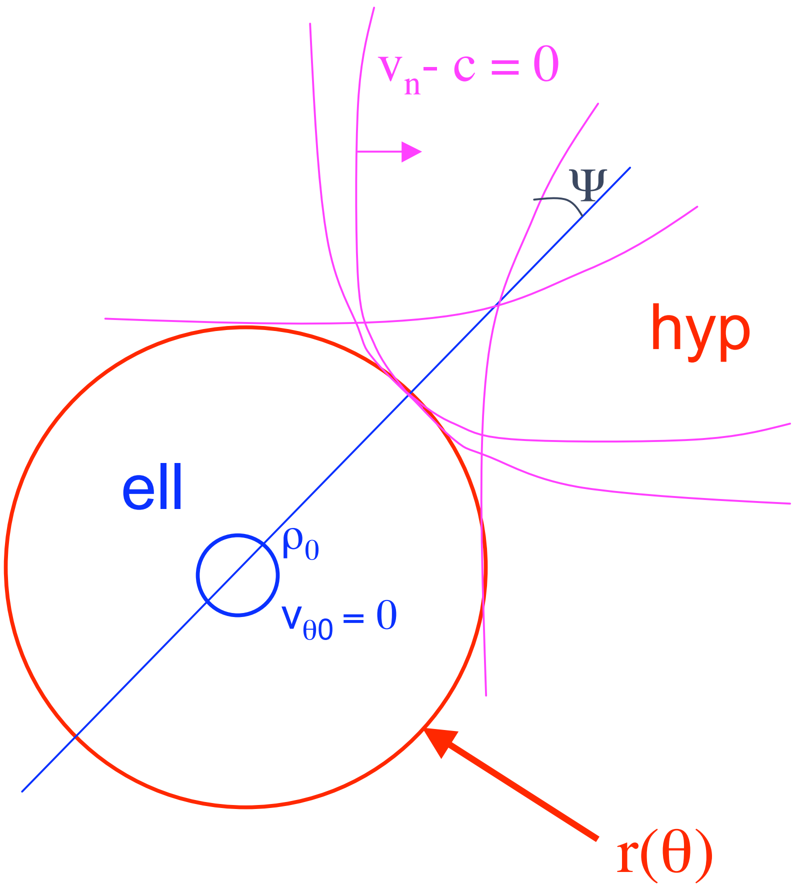
Extension to 2D, 3D: critical curves

$\sin \Psi = 1 / M$



ρ_0

no u_0!



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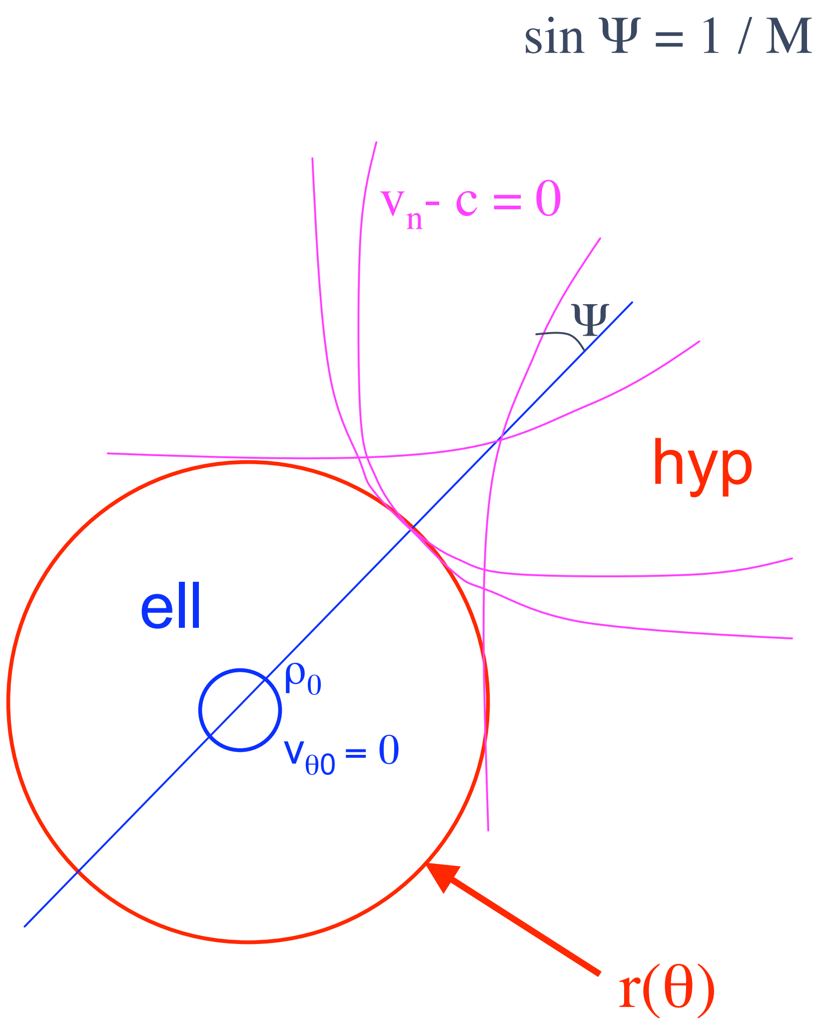
Extension to 2D, 3D: critical curves

- assume isothermal flow:
  ρ, u, v
- simple case: $v_\theta = 0$
- critical curve
  = transition from subsonic to supersonic
  = transition from elliptic to hyperbolic
  = limiting line for the characteristics
  (envelope of characteristics, $v_n - c = 0$)
- guess critical curve: $r(\theta)$
- discretize: $r_i = r(\theta_i)$
- solve PDE using (nonlinear) FD method in smooth region inside critical curve
- adjust r_i until boundary conditions are satisfied (1D Newton procedure on $F(r_i)=0$, dense matrix)



Extension to 2D, 3D: critical curves

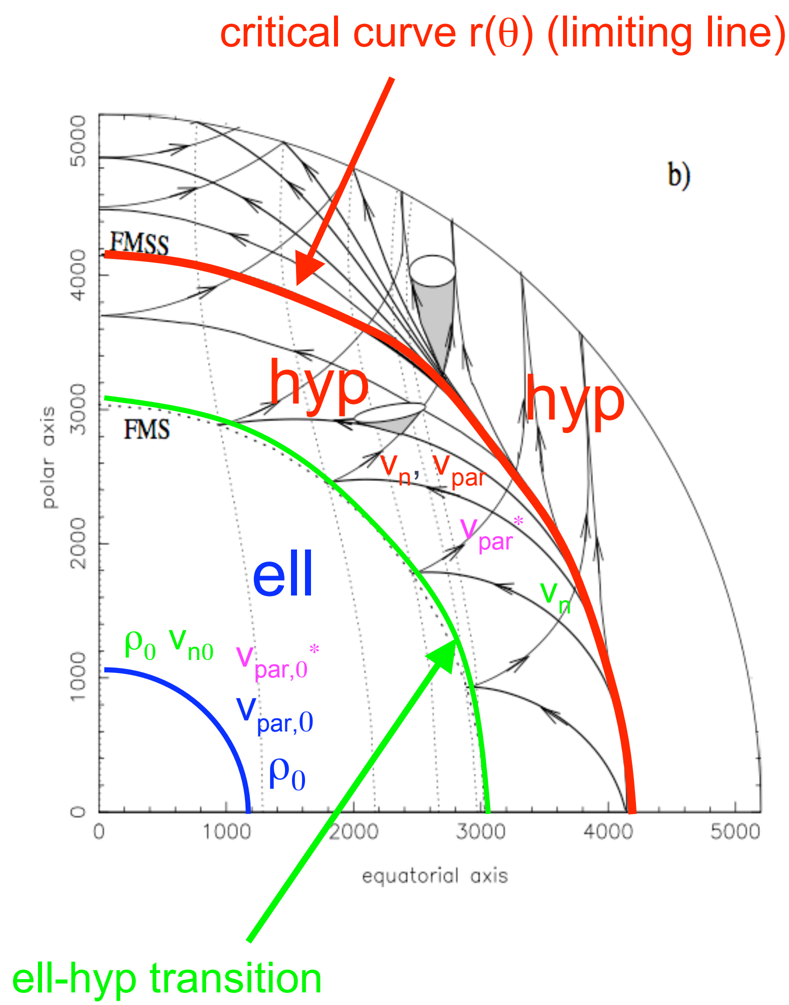
- assume isothermal flow: ρ, u, v
- general case: $v_\theta \neq 0$
- critical curve

  = limiting line for the characteristics (envelope of characteristics, $v_n - c = 0$)
- critical curve

  $\neq$ transition from subsonic to supersonic,

  = transition from elliptic to hyperbolic

  $(v_{tot} - c = 0)$
- guess critical curve: $r(\theta)$, gives v_n, v_{par}, guess v_{n0}
- solve PDE using (nonlinear) FD method in smooth region inside critical curve (can integrate through ell-hyp boundary), with BC $v_n\ \rho_0\ v_{n0}$, this gives $v_{par,0}^*$, v_{par}^*
- adjust r_i and v_{n0} until $v_{par,0} = v_{par,0}^*$, $v_{par} = v_{par}^*$ (1D Newton procedure on $F(r_i, v_{n0})=0$, dense matrix)



hdesterck@uwaterloo.ca

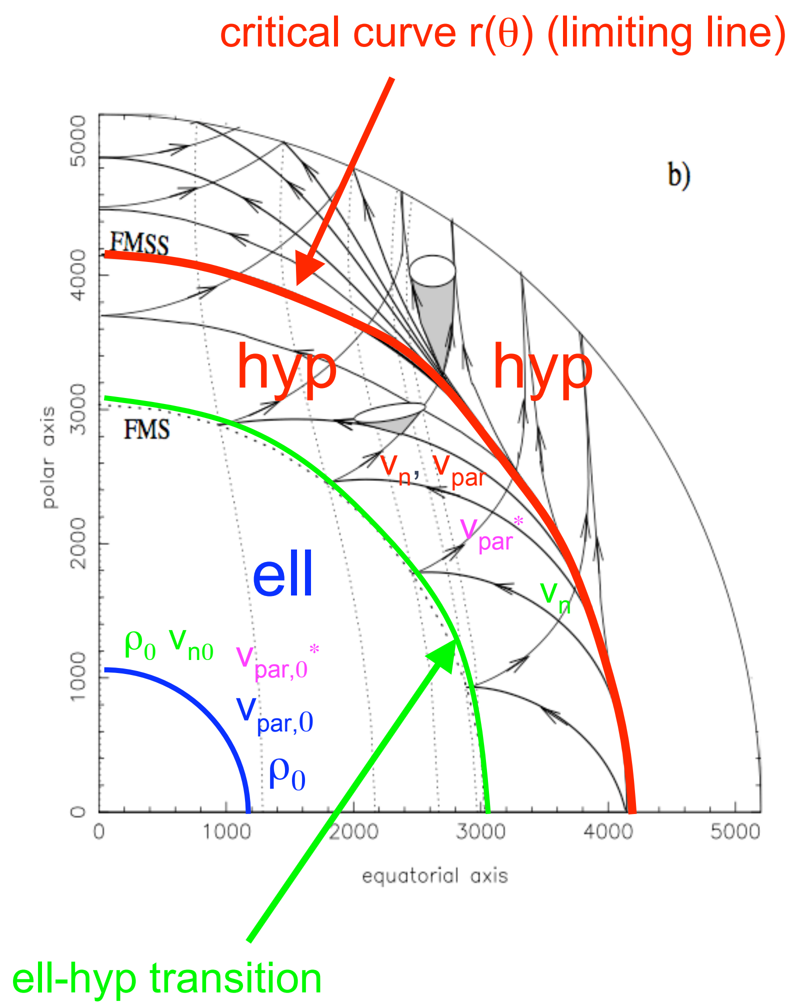
Extension to 2D, 3D: critical curves

- guess critical curve: $r(\theta)$, gives v_n, v_{par}
- guess v_{n0}
- discretize: $r_i=r(\theta_i)$
- solve PDE using (nonlinear) FD method in smooth region inside critical curve (can integrate through ell-hyp boundary), with BC

  v_n ρ_0 v_{n0} , this gives $v_{par,0}^*$, v_{par}^*
- adjust r_i and v_{n0} until $v_{par,0}= v_{par,0}^*$, $v_{par}= v_{par}^*$ (1D Newton procedure on

  $F(r_i, v_{n0})=0$, dense matrix)

- open problems:
  - how to derive v_n, v_{par} from limiting line condition
  - how to continuate solution from limiting line (dynamical system?)



7. Conclusions

- solving steady Euler equations directly is superior to time-marching methods for 1D transonic flows
- NCP uses
  - adaptive integration outward from critical point
  - dynamical system formulation
  - 2x2 Newton method to match critical point with BC
- 1D: so what?
  - can use inefficient methods (?)
  - there are real 1D applications!

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hdesterck@uwaterloo.ca

1D applications: exoplanet and early earth

THE ASTROPHYSICAL JOURNAL, 621:1049–1060, 2005 March 10

TRANSONIC HYDRODYNAMIC ESCAPE OF HYDROGEN FROM EXTRASOLAR PLANETARY ATMOSPHERES

FENG TIAN,[1,2] OWEN B. TOON,[2,3] ALEXANDER A. PAVLOV,[2] AND H. DE STERCK[4]

13 MAY 2005 VOL 308 SCIENCE www.sciencemag.org

A Hydrogen-Rich Early Earth Atmosphere

Feng Tian,[1,2*] Owen B. Toon,[2,3] Alexander A. Pavlov,[2] H. De Sterck[4]

Conclusions

- 2D, 3D, time-dependent: future work
  - integrate separately in different domains of the flow, ‘outward’ from critical curves
  - match conditions at critical curves with BCs using Newton method
  - issues:
    - change of topology (level sets?)
    - solve nonlinear PDEs in different regions (cost?)
    - smaller but dense Newton system
    - conditions at limiting lines and continuation?
    - time-dependent (do the same in space-time?)

hdesterck@uwaterloo.ca

Conclusions

- 2D, 3D, time-dependent : future work
  - issues:
    - change of topology (level sets?)
    - solve nonlinear PDEs in different regions (cost?)
    - smaller but dense Newton system
    - conditions at limiting lines and continuation?
    - time-dependent (do the same in space-time?)
  - potential advantages are significant: problem more well-posed
    - fixed number of Newton steps, linear iterations (scalable)
    - better grid sequencing (nested iteration)
    - can use simple high-order methods in smooth flow, no limiters (which are a headache)

hdesterck@uwaterloo.ca

Thank you

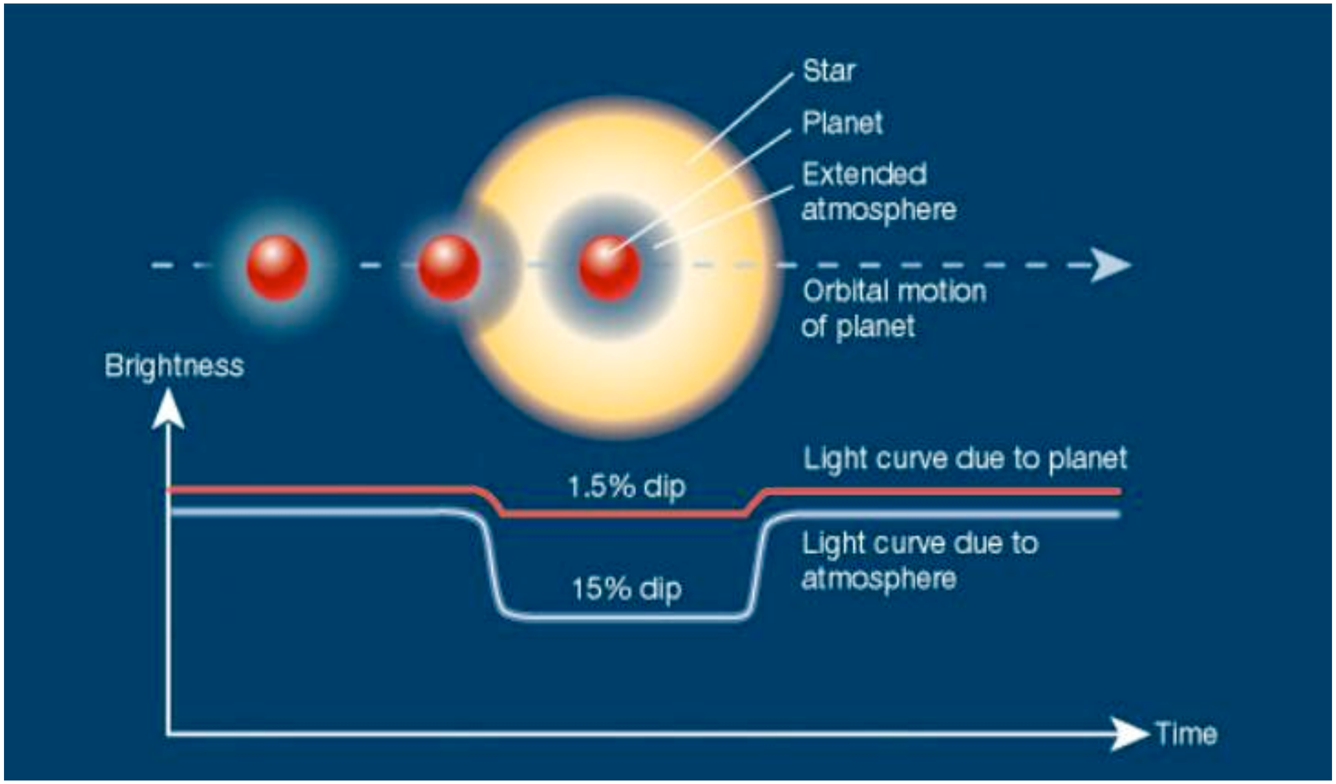
hdesterck@uwaterloo.ca

Overview

1. Motivation and context
2. 1D model problems (ODE systems)
3. Newton Critical Point (NCP) method for ODE steady transonic Euler flows
4. Extension to problems with shocks
5. Extension to problems with heat conduction
6. Extension to 2D, 3D
7. Conclusions

hdesterck@uwaterloo.ca

Transiting exoplanet



hdesterck@uwaterloo.ca