Numerical methods for nonlinear ODE and PDE systems that describe stationary transonic fluid flow

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Applied Mathematics Colloquium
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this presentation is about ...

- stationary compressible fluid flows
- flow solutions with transitions from subsonic to supersonic regions separated by critical points and shocks
- efficient numerical simulation methods for such flow solutions
- PDEs (multi-D) and ODEs (1D)
- some elements of dynamical systems
- applications: solar wind, nozzle flows, black hole accretion, exoplanets, early earth atmosphere, ...

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Overview

1. Stationary transonic fluid flow
2. Numerical simulation using time marching
3. Solving the stationary equations directly (ODE)
   I. Isothermal case
   II. Full Euler case
   III. Shocks
   IV. Heat conduction
4. An application
5. Extension of numerical method to 2D (PDE)
6. Some further potential applications

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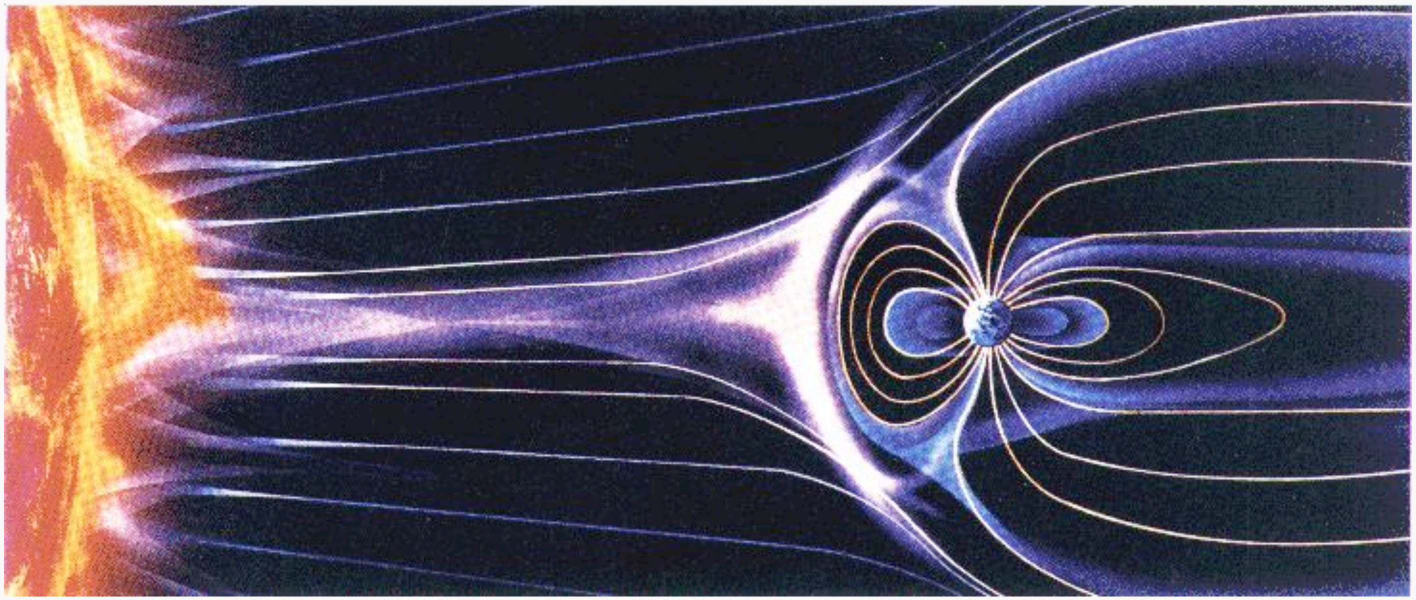
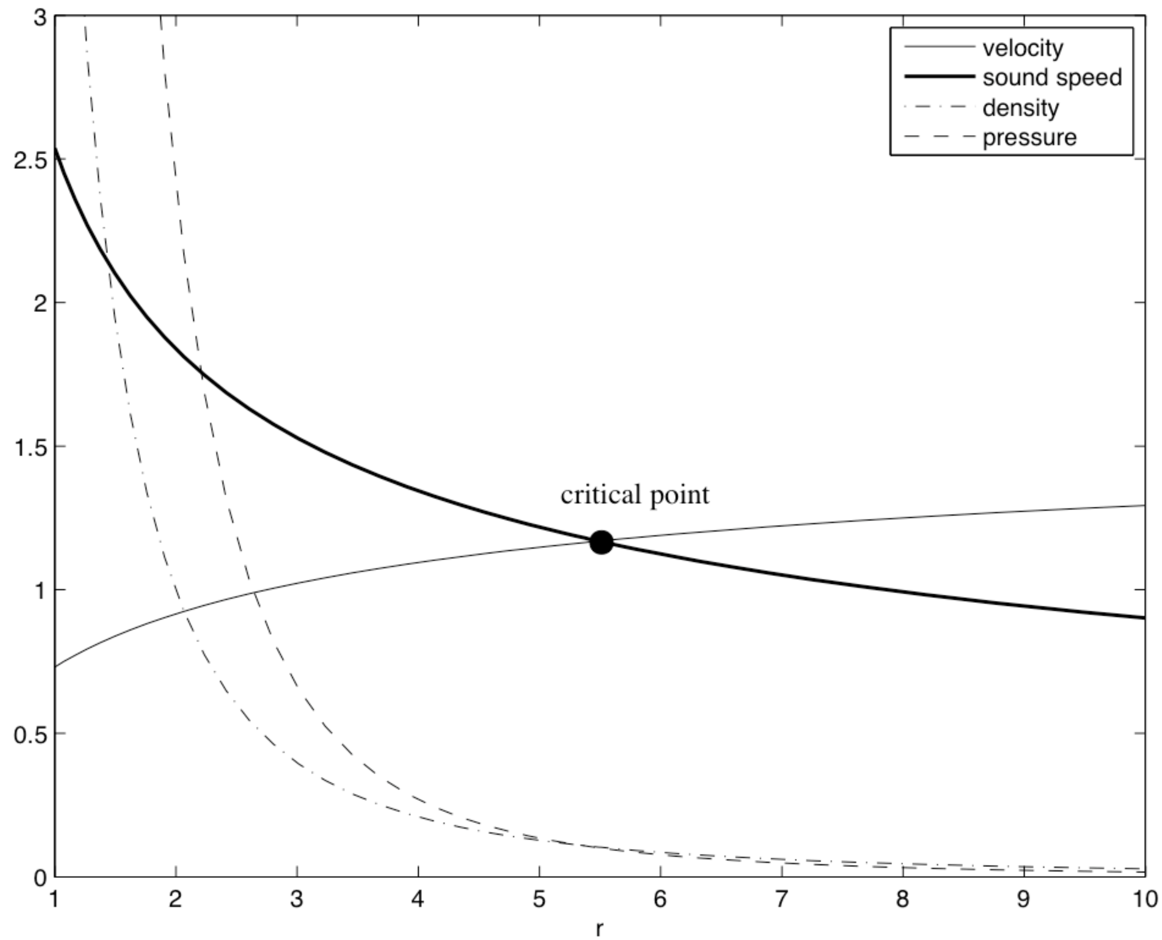
1. Stationary transonic fluid flow

- example: solar wind



Parker's solar wind model



subsonic ⇒|⇐ supersonic

1D Compressible Euler equations (radial)

- time-dependent (nonlinear PDE system):

  find $\rho(r,t), u(r,t), p(r,t)$ s.t.

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

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

- hyperbolic system, wave speeds $u, u+c, u-c$

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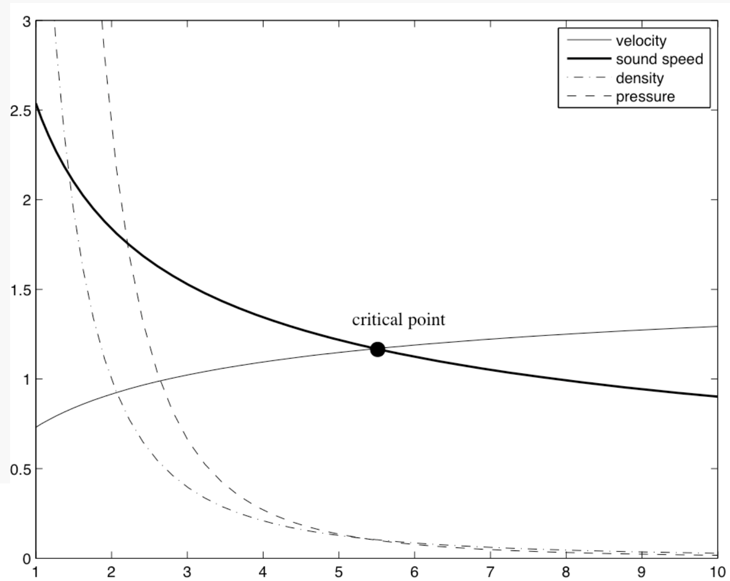
1D Compressible Euler equations (radial)

- stationary (nonlinear ODE system):

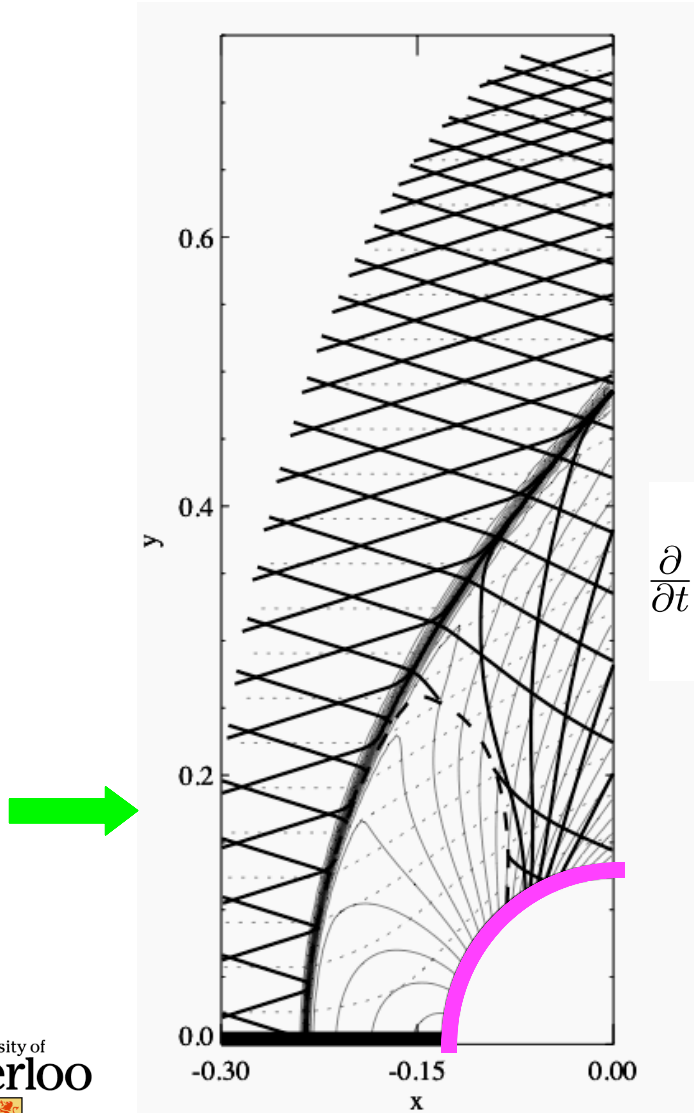
  find $\rho(r), u(r), p(r)$ s.t.

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



subsonic $\Rightarrow |^{r} \Leftarrow$ supersonic

2D Compressible Euler equations



- find

$$\rho(x,y,t), v_x(x,y,t),$$
$$v_y(x,y,t), p(x,y,t)$$

s.t.

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

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

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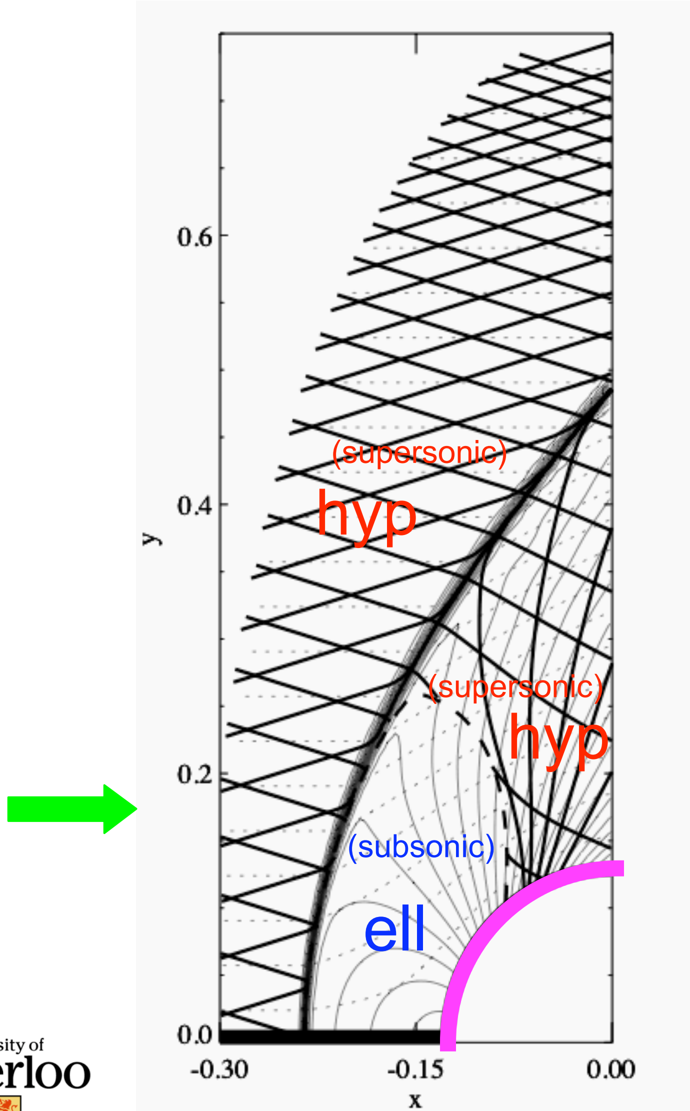
2D Compressible Euler equations



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

- stationary flow:

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

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

- transition from supersonic to subsonic flow at shock and critical curve

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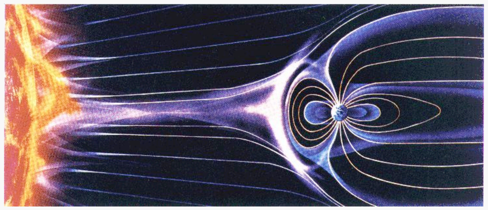
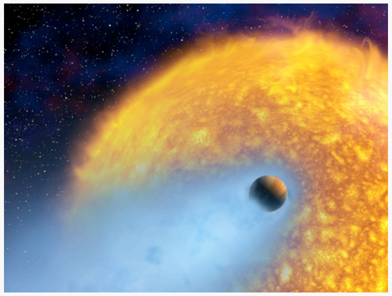
Applications

- solar wind



- extrasolar planets



- aerodynamics

- ...

2. Numerical simulation using time marching

- march initial condition toward steady state in time

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

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

- often implicit time integration
- use, for example, finite volume method
- nonlinear: perform Newton linearization

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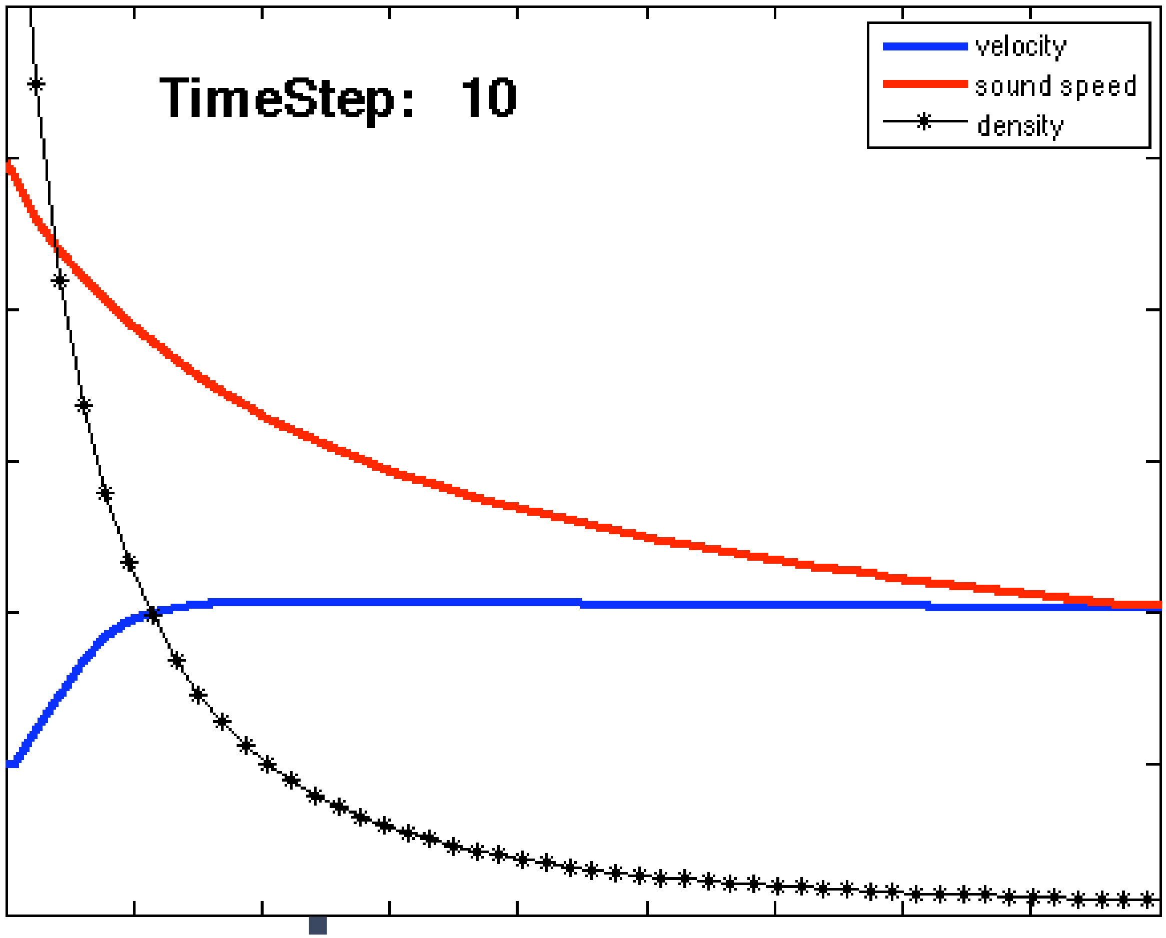
Numerical simulation using time marching

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

- advantages of this approach:
  - use more 'simple' hyperbolic boundary conditions
  - 'physical' initial guess for Newton
  - it works!
- problems with this approach:
  - it works, but (very) slow convergence to steady state
  - does not scale well: computational work (Newton iterations, ...) grows very fast as a function of resolution (much faster than O(n))
  - robustness

Use time marching method (explicit)



u - c = 0

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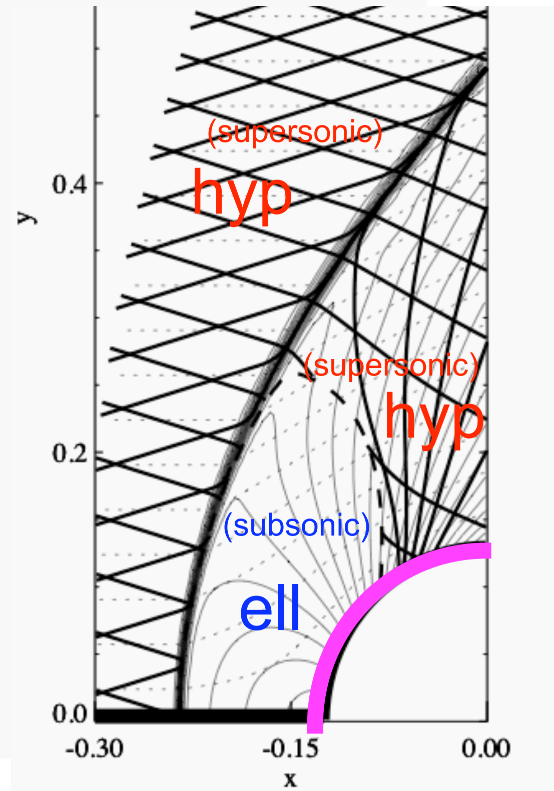
Why not solve the steady equations directly?

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

- 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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3. Solving the stationary equations directly (ODE)

- stationary Euler, radial:

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

- simplified system: isothermal Euler (T=constant)

find $u(r),\ \rho(r)$ s.t.

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

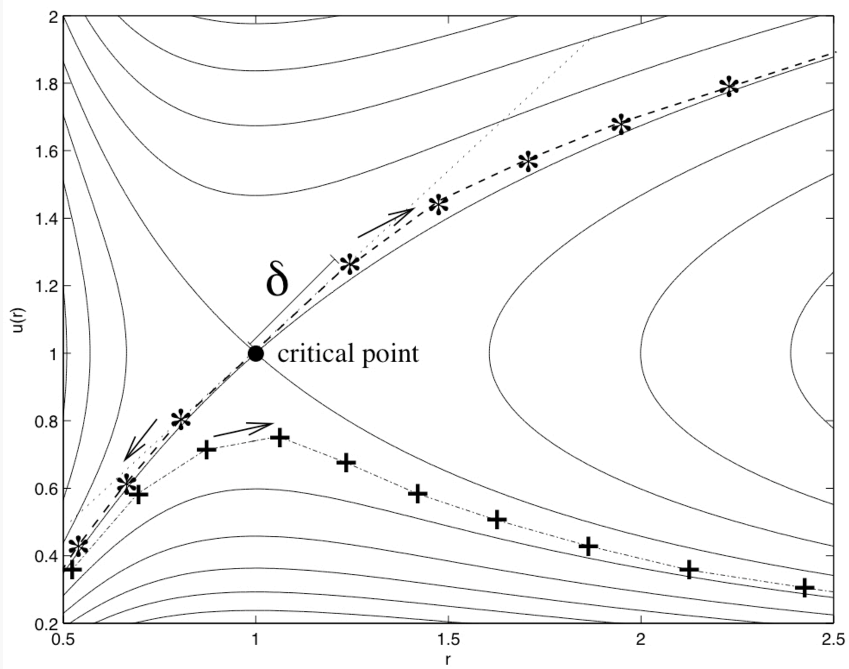
$$\frac{du}{dr} = \frac{2\, u\, c^2\, (r - r_c)}{r^2\, (u^2 - c^2)}$$

3.I Isothermal case

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

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

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



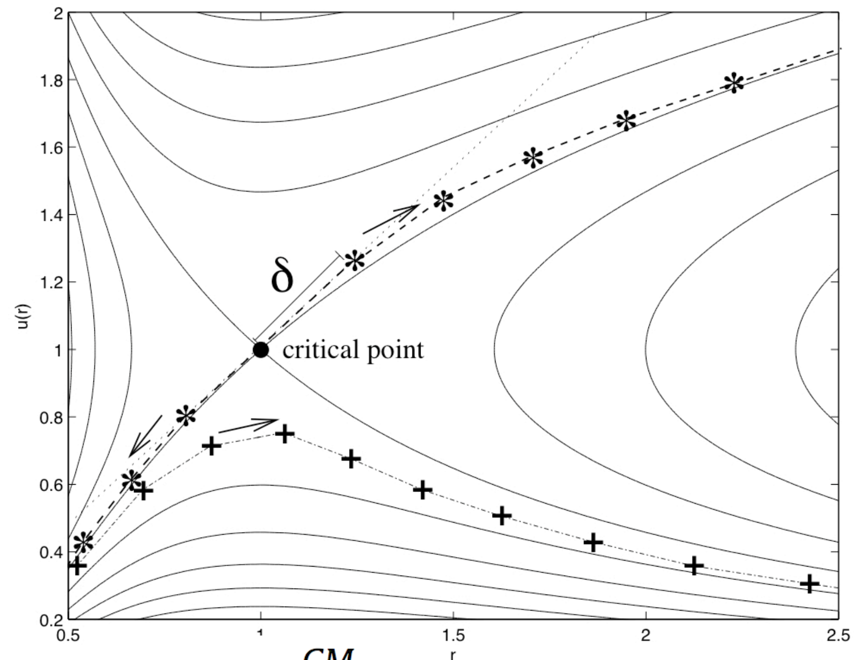
- critical point:
  - du/dr is undefined
  - equilibrium point of associated dynamical system

Solving the ODE system numerically 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 numerically 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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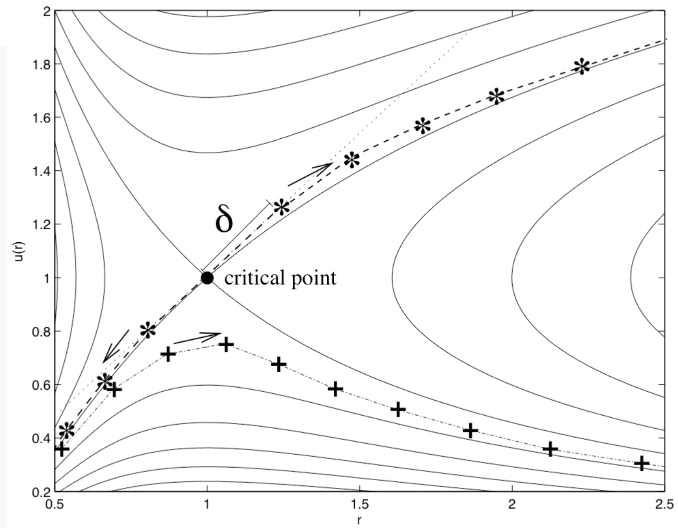
Solution: integration outward from critical point

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

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

3.II Full Euler case (T not constant)

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

- 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)

Full Euler dynamical system

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

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

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

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

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

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

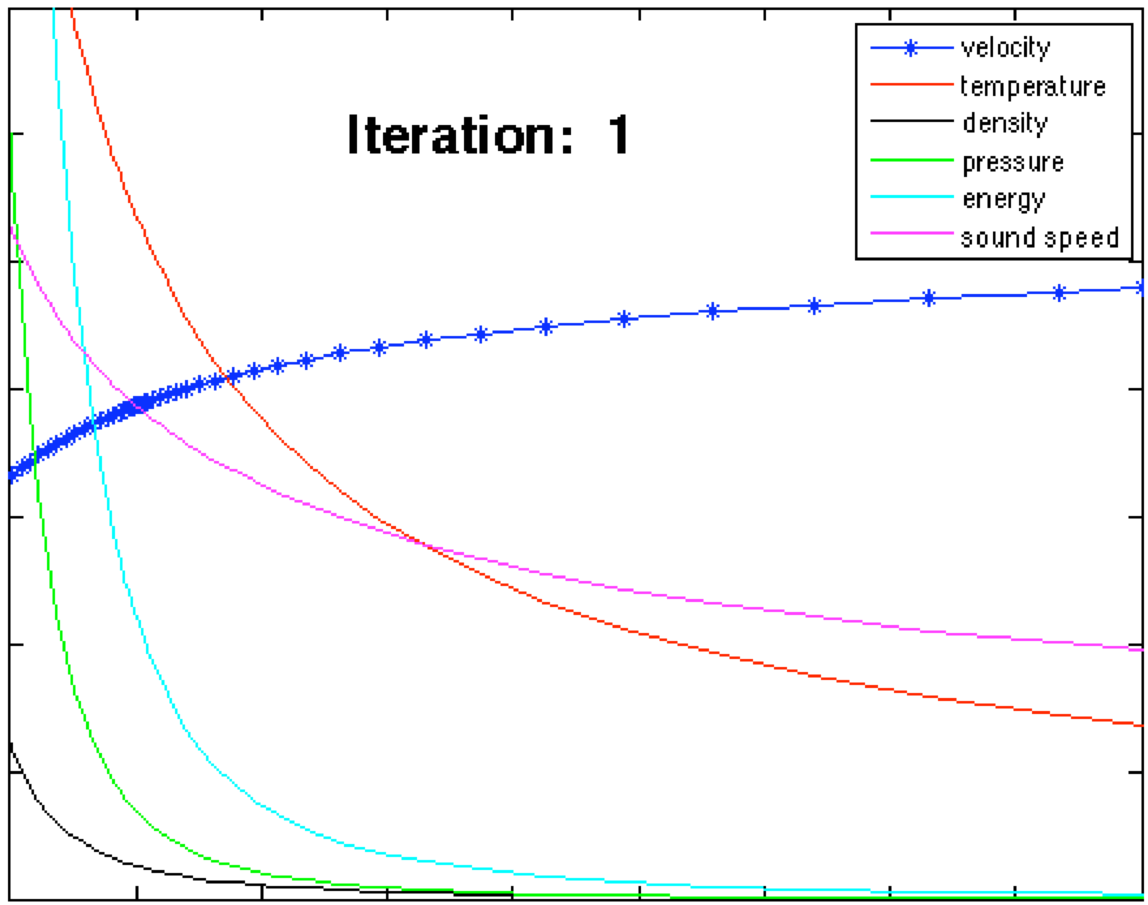
Newton Critical Point (NCP) method: use Newton method to match critical point with BCs

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

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



ρ_0

p_0

u_0

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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

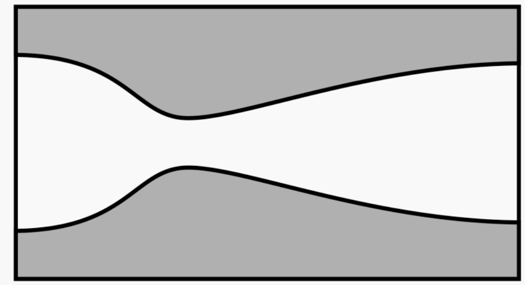
Journal of Computational and Applied Mathematics 223 (2009) 916–928

A fast and accurate algorithm for computing radial transonic flows

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

3.III Extension to problems with shocks

- consider quasi-1D nozzle flow



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

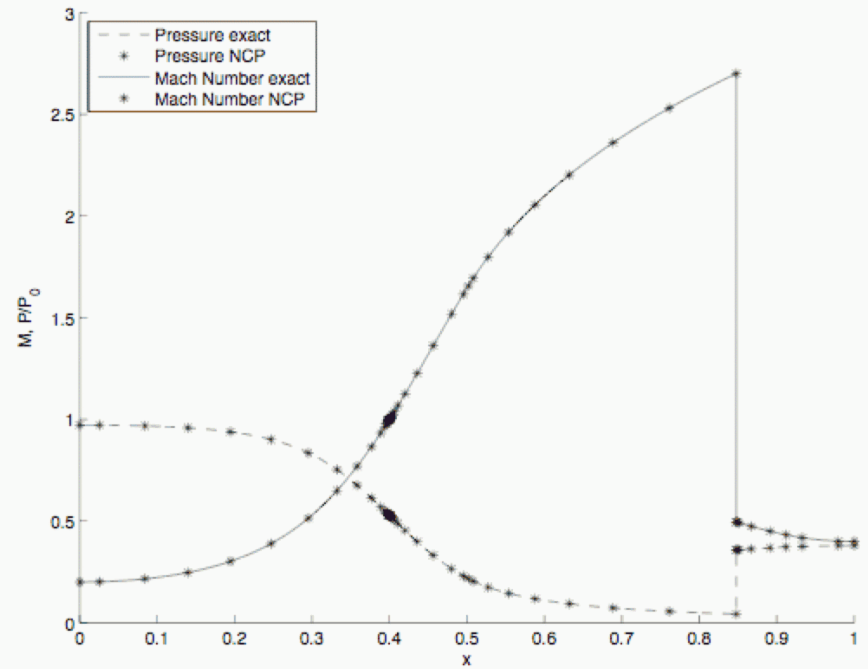
$$\Rightarrow \quad \begin{aligned} u_{crit} &= \sqrt{\gamma\, T_{crit}} = c_{crit}, \\ \frac{dA}{dx}(x_{crit}) &= 0. \end{aligned}$$

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)



at shock:

$$F(U_l) = F(U_r)$$

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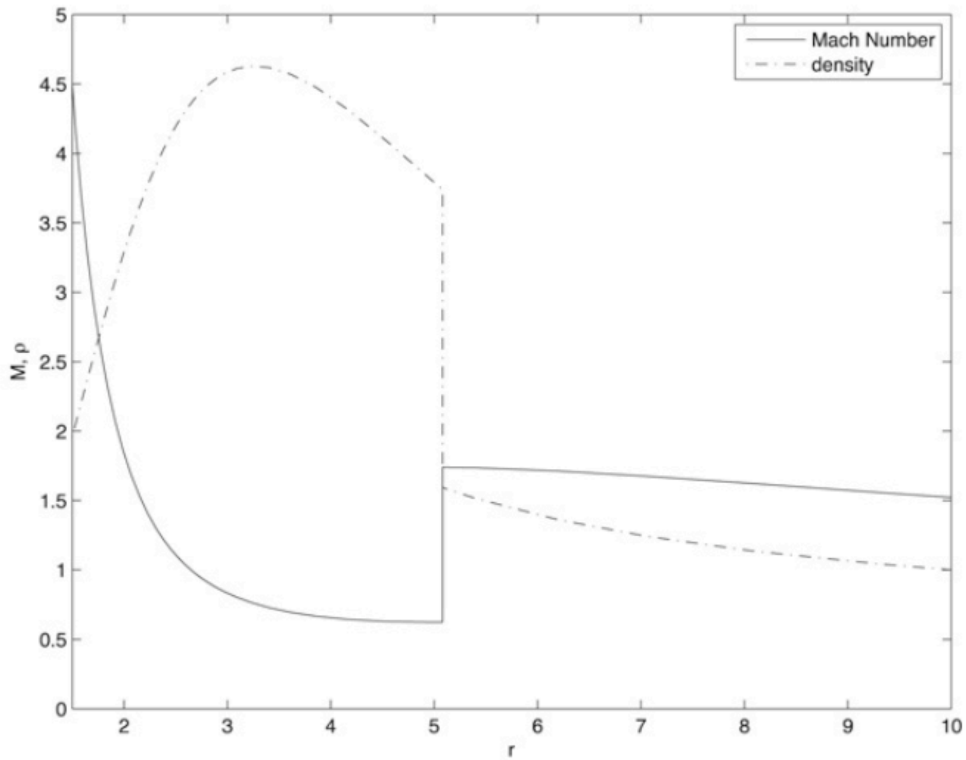
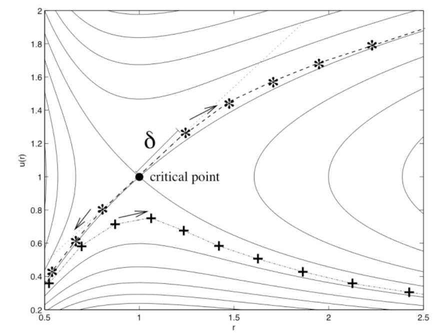
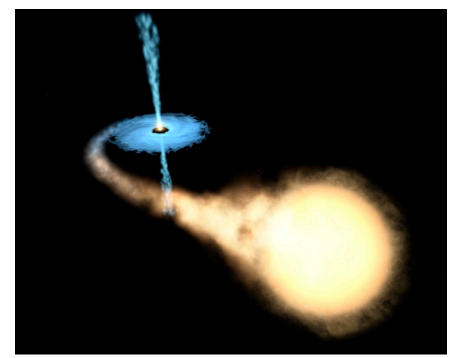
Other application: black hole accretion







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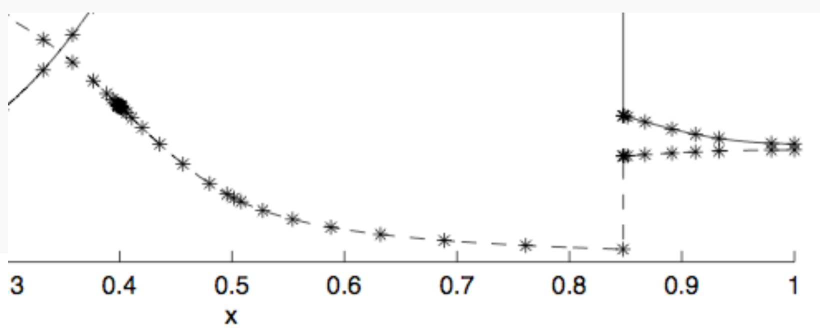
Some thoughts

- it is hard to find numerical approximations of discontinous functions without oscillations (Gibbs ...)
- ingenious methods have been invented attempting to obtain monotone solutions for nonlinear PDEs (using 'limiters' etc. ...)
- NCP gives monotone solution, 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
- this is 1D... would be nice if we could do something like this in 2D, 3D, time-dependent!



3.IV 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†

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

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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Two critical points of different type!

- sonic critical point (node):

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

- thermal critical point (saddle point):

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

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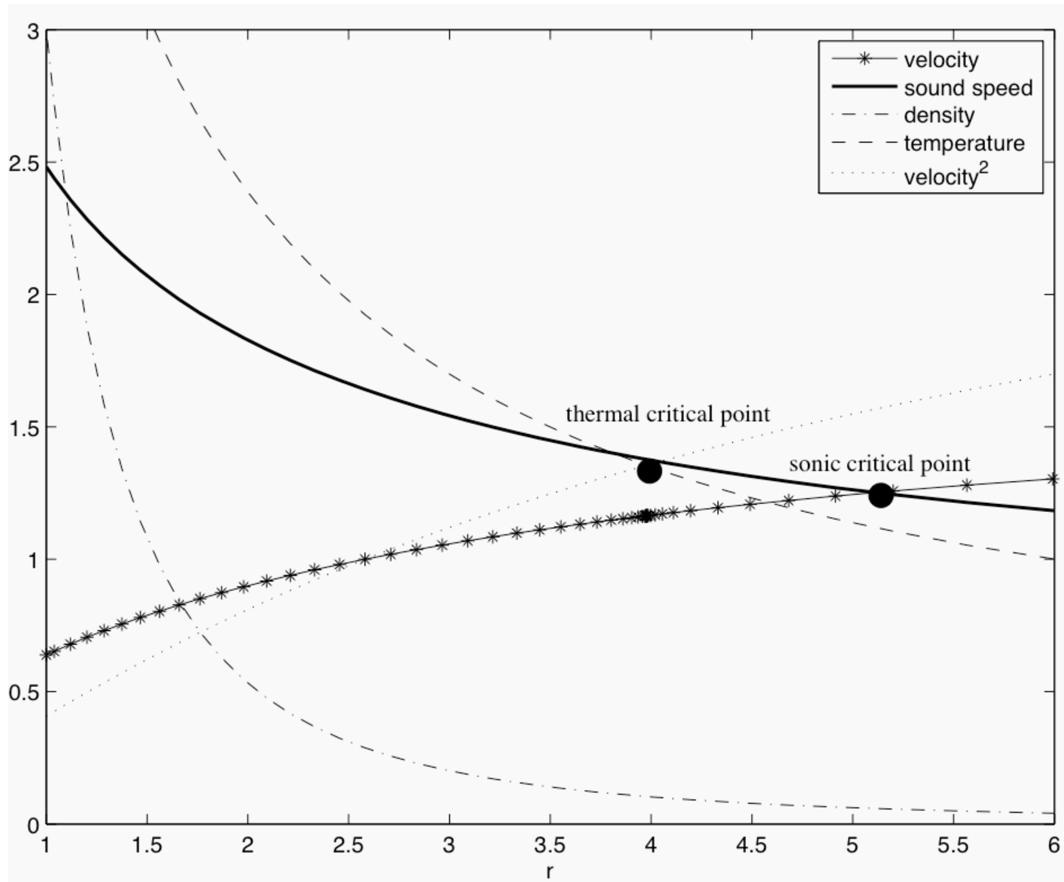
Transonic flow with heat conduction

- 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



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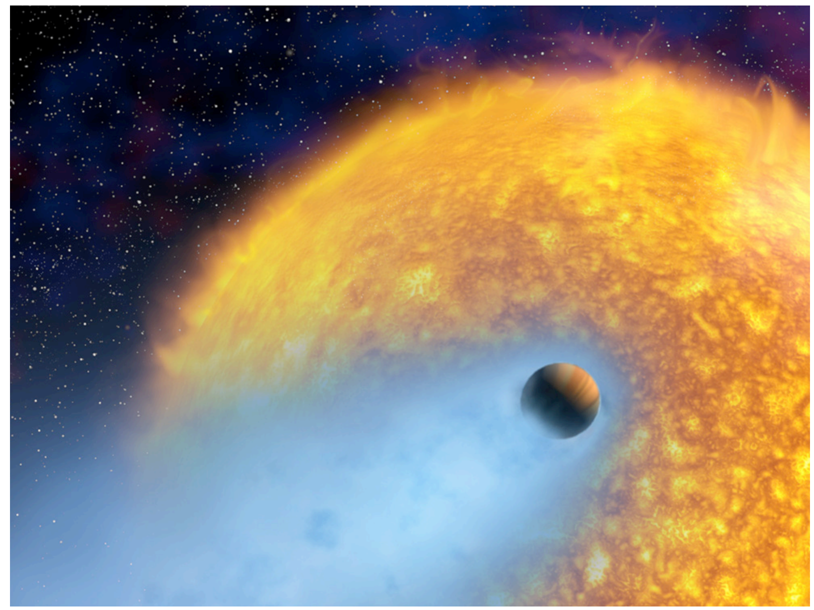
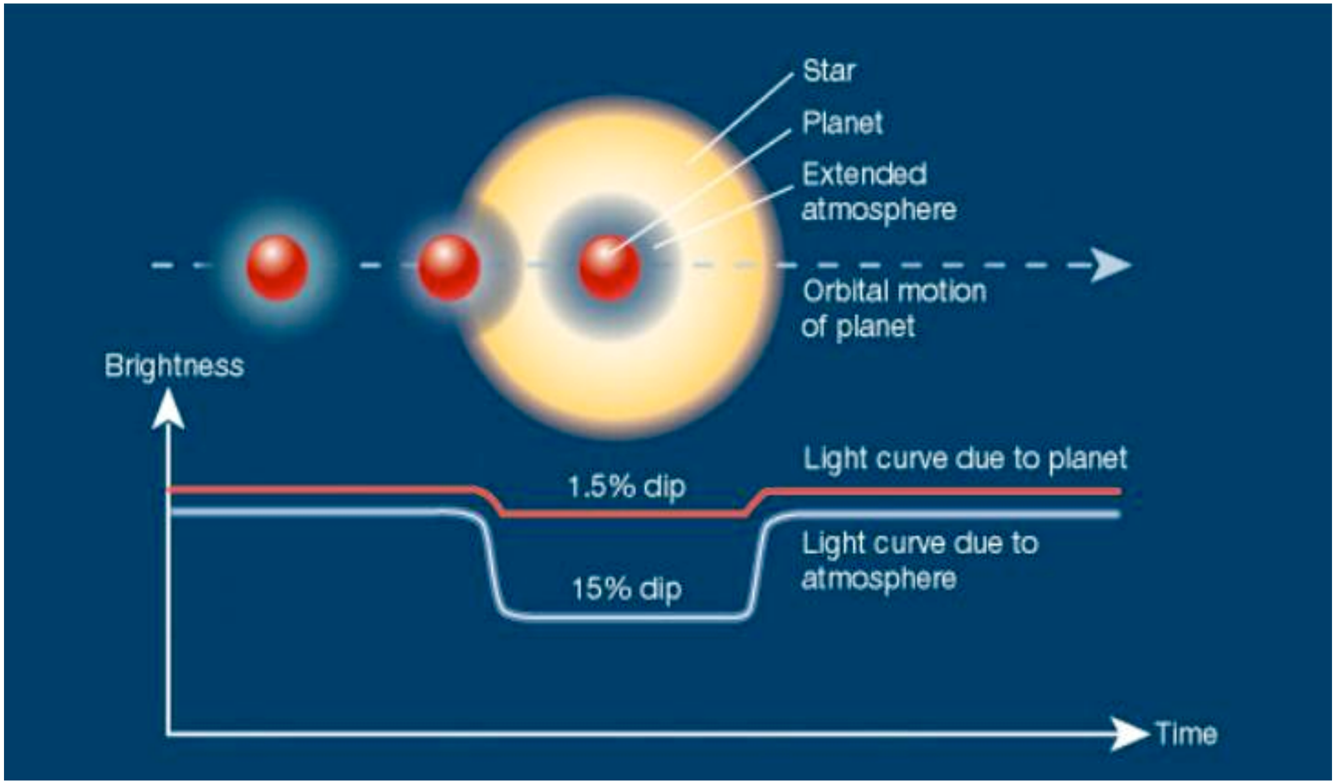
4. An application: radial outflow from exoplanet

- http://exoplanet.eu
- 403 extrasolar planets known, as of November 2009
- 42 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



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? ⇒ solve Euler equations!

results for 1D exoplanet simulations

- HD209458:
  - 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 ⇒ HD209458b is stable

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

TRANSONIC HYDRODYNAMIC ESCAPE OF HYDROGEN FROM EXTRASOLAR PLANETARY ATMOSPHERES

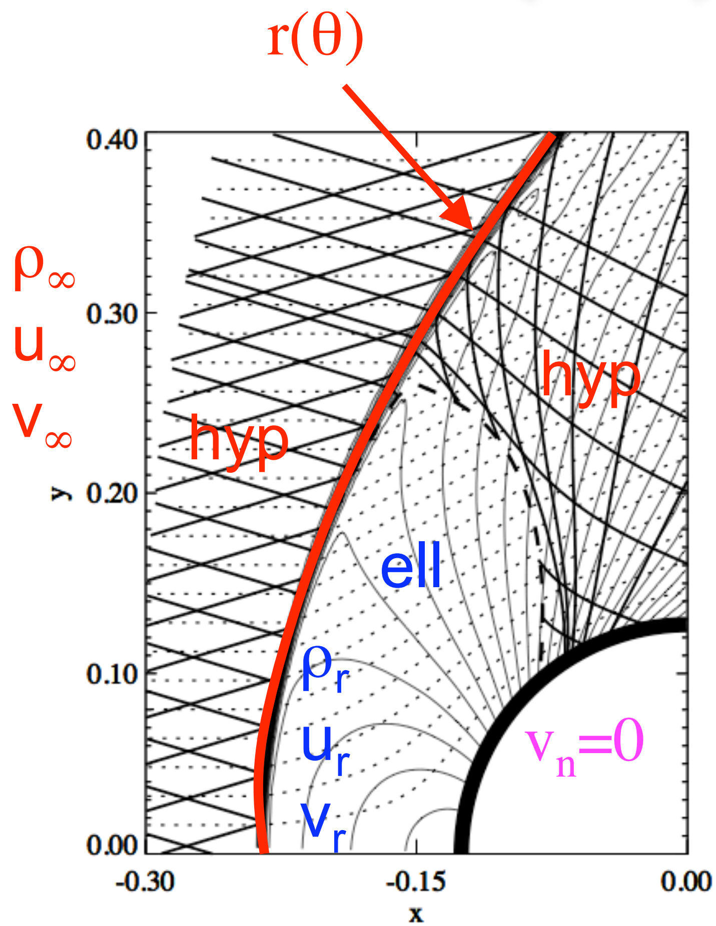
FENG TIAN,[1,2] OWEN B. TOON,[2,3] ALEXANDER A. PAVLOV,[2] AND H. DE STERCK[4]

5. Extension of numerical method to 2D (PDE)

- 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!



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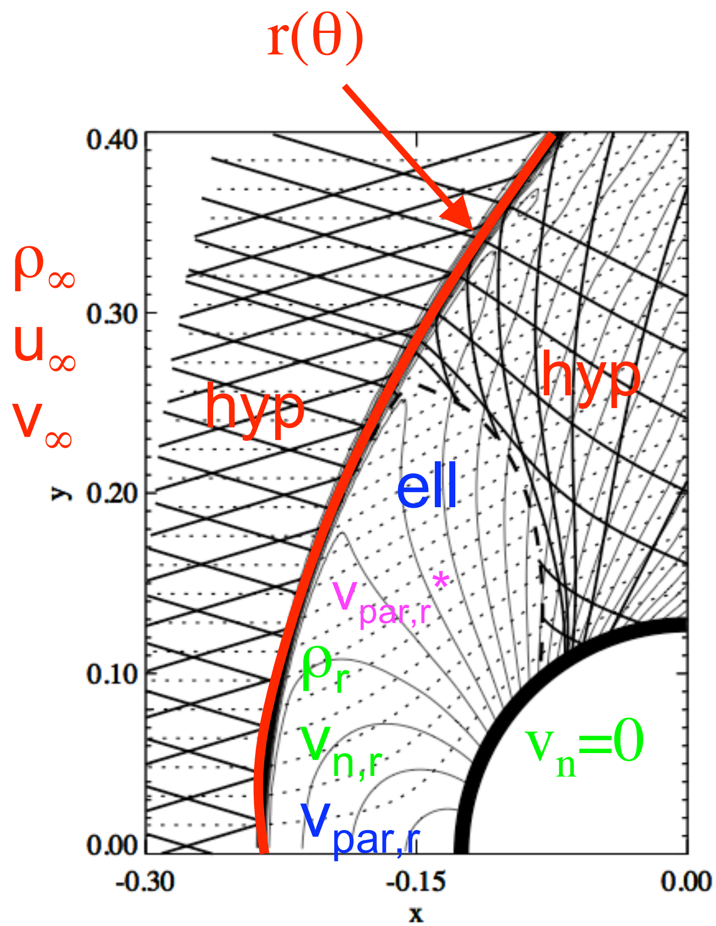
bow shock flows

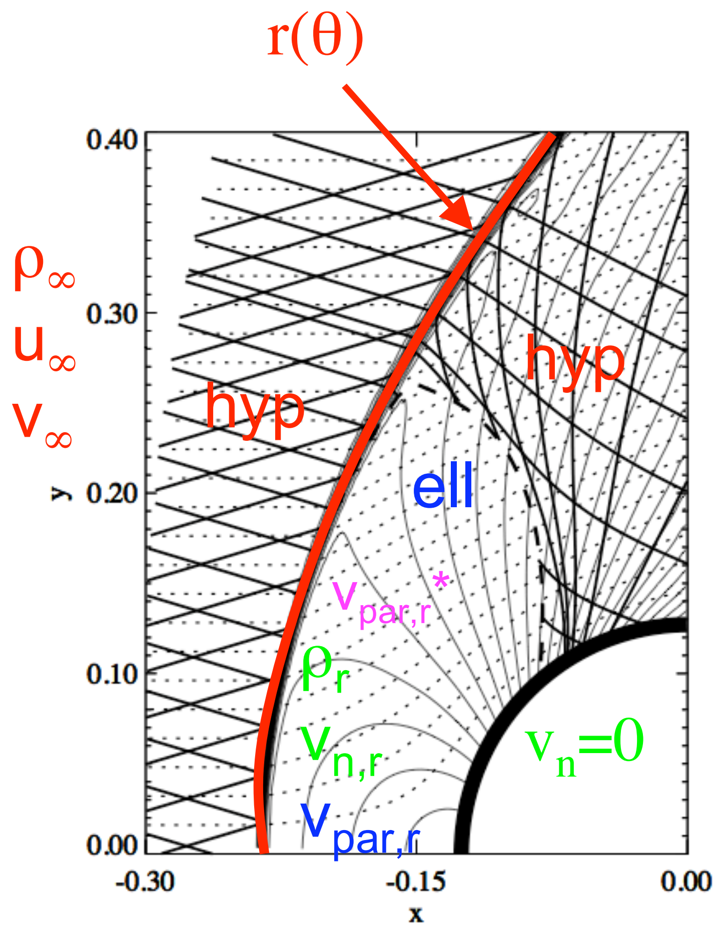
- solution: solve PDE using (nonlinear) FD method in smooth region on right of shock, with BC ρ_r, $v_{n,r}$, $v_{par,r}=0$, this gives $v_{par,r}^*$

- adjust r_i until $v_{par,r}^* = v_{par,r}$ at shock (1D Newton procedure on $F(r_i)=0$, dense matrix)



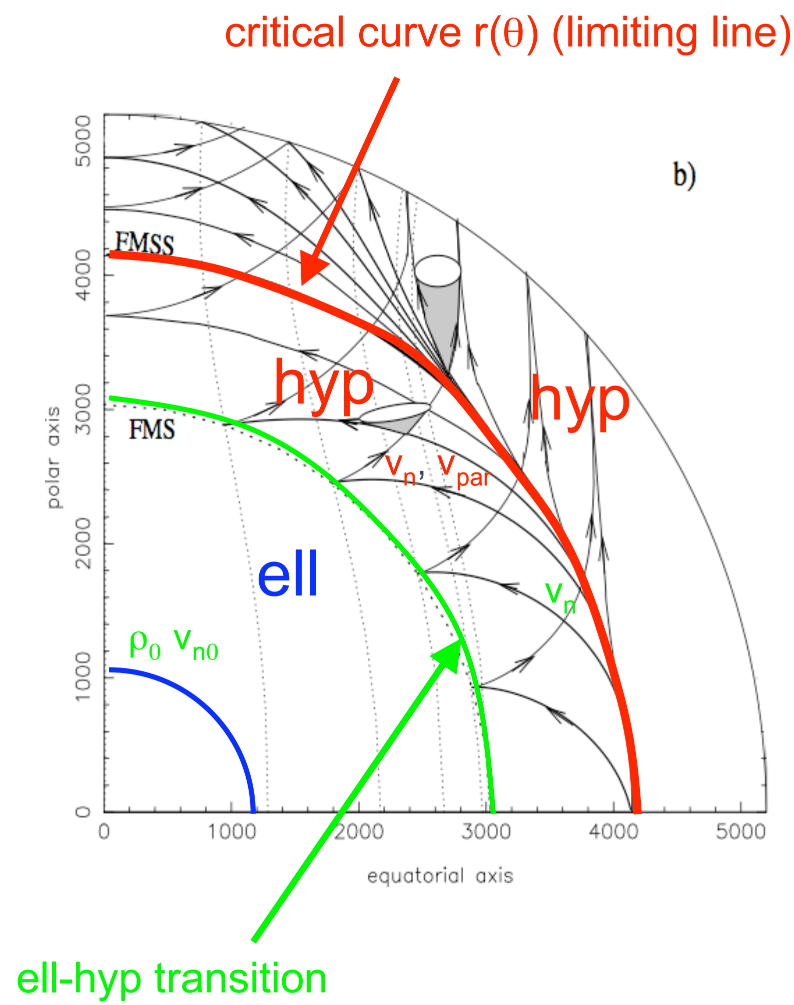
bow shock flows

- 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
- efficiency?; robustness?



Extension to 2D, 3D: critical curves

- critical curves appear much harder to handle
- 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: $r(\theta)$, but how to relate flow quantities to limiting line position?
- open problems:
  - how to derive v_n, v_{par} from limiting line condition
  - how to continuate solution from limiting line (dynamical system?)



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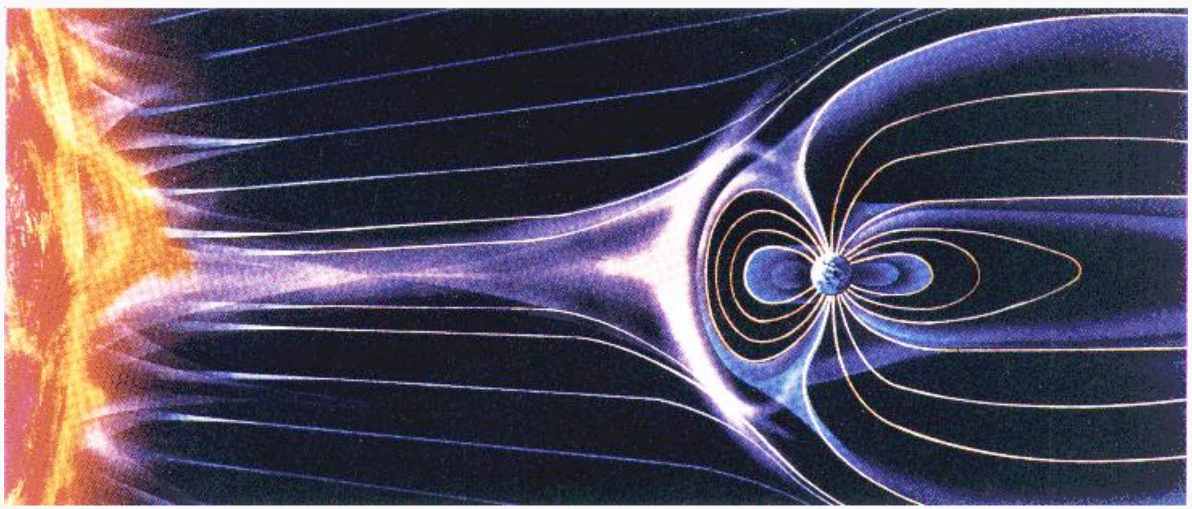
6. Some further potential applications

(1) "Solar Drivers of Space Weather: Contributions to Forecasting" (project funded by CSA, 2009-2012)

- Lucian Ivan (postdoc)
- 3D simulation of solar wind, coronal mass ejections
- ultimate goal: "predict Space Weather"



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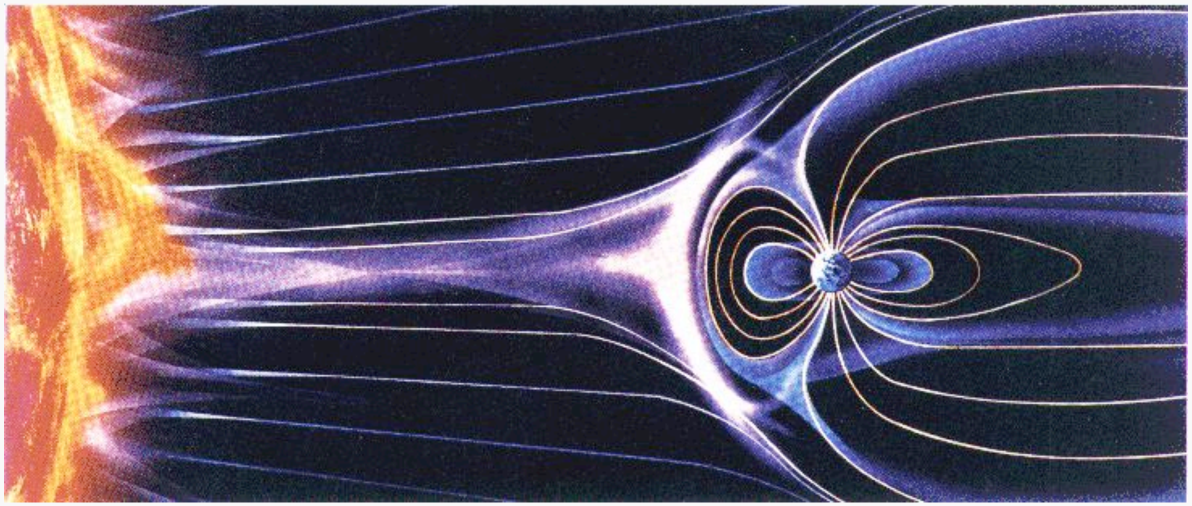
Solar wind simulation

- “cubed sphere” block-adaptive high-order MHD code
- for now, we use time marching for calculating 3D solar wind
- collaboration with Prof. Groth, UofT Aerospace Eng.
- but ... perhaps 3D version of NCP can be developed



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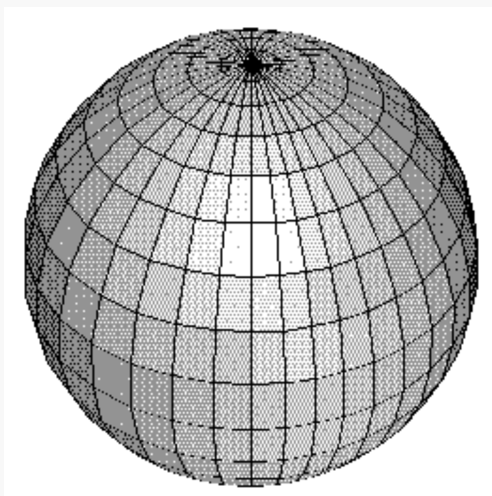
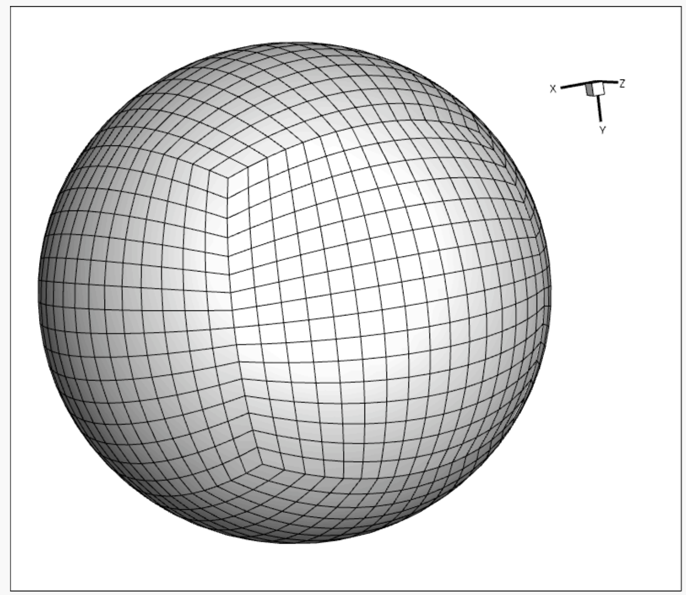
Solar wind simulation

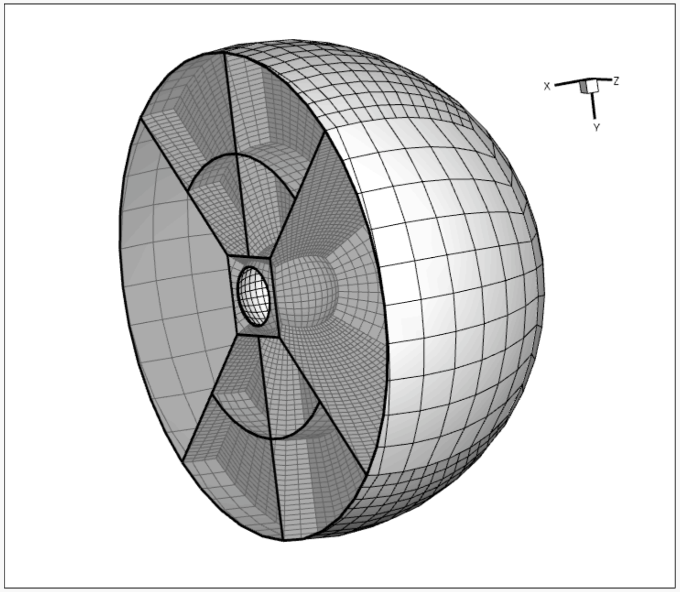
- “cubed sphere” block-adaptive high-order MHD code

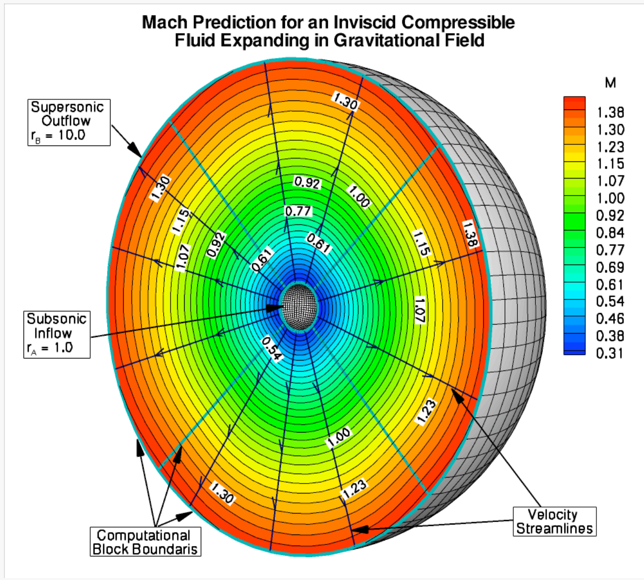




Solar wind simulation

- “cubed sphere” block-adaptive high-order MHD code





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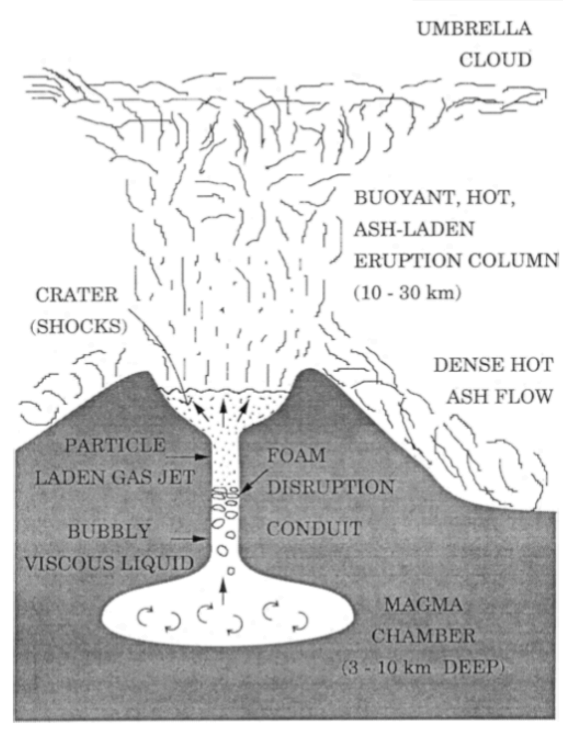
Some further potential applications

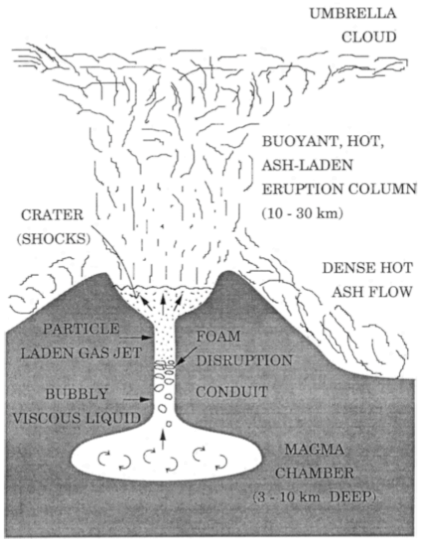
(2) THE DYNAMICS OF EXPLOSIVE VOLCANIC ERUPTIONS

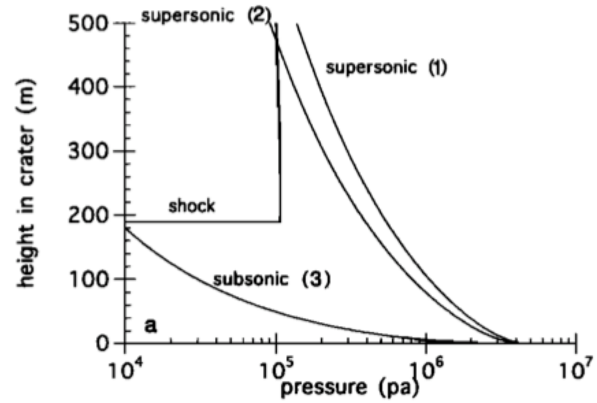
Andrew W. Woods
Institute of Theoretical Geophysics
Cambridge, England

Reviews of Geophysics, 33, 4 / *November 1995*
pages 495–530



Explosive volcanic eruptions





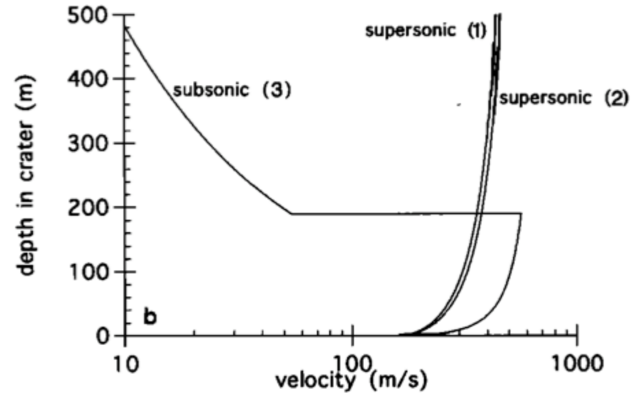


Figure 8. (a) Pressure and (b) velocity profiles of a jet decompressing in a crater. In flow 1 the vent pressure is approximately 45 atm, and the flow remains overpressured all the way to the top of the crater and therefore issues as a supersonic jet. In flow 2 the vent pressure is smaller, and the flow becomes underpressured in the crater but still issues as a supersonic jet. In flow 3 the vent pressure is only of the order of 20 atm, and the flow becomes so underpressured in the crater that a shock forms, and a very slow subsonic jet issues from the vent.

thank you... questions?

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