Supersonic Planetary Flow Simulations and the Origin of Life

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Collaborators

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Do you know how to solve these equations...

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

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

- Euler Equations of Gas Dynamics
- conservation of mass, momentum, energy
Do you know how to solve these equations?

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

\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho r^2 \\ \rho u r^2 \\ \left( \frac{p}{\gamma - 1} + \frac{\rho u^2}{2} \right) r^2 \end{bmatrix} + \frac{\partial}{\partial r} \begin{bmatrix} \rho u r^2 \\ \rho u^2 r^2 + p r^2 \\ \left( \frac{\gamma p}{\gamma - 1} + \frac{\rho u^2}{2} \right) u r^2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -\rho G M + 2 p r \end{bmatrix}
\]

- Nonlinear Partial Differential Equation System, of “hyperbolic” type
- assumes spherical symmetry, radial motion
Euler Equations of Gas Dynamics

- describe compressible gases
- describe waves in gases: sound waves
- when the sound source moves... :

\[
\begin{array}{c|c|c}
\text{(a) static} & \text{(b) subsonic} & \text{(c) supersonic} \\
\begin{array}{ccc}
\text{\(v = 0\)} \\
\text{\(- c \quad \bullet \quad + c\)} \\
\end{array} & \begin{array}{ccc}
\text{\(v - c\)} & \text{\(v + c\)} \\
\text{\(v \ (\ < \ c \ )\)} \\
\end{array} & \begin{array}{ccc}
\text{\(v - c\)} & \text{\(v + c\)} \\
\text{\(v \ (\ > \ c \ )\)} \\
\end{array}
\end{array}
\]

- analogy: small perturbation in a moving river
Application 1: Aerospace Engineering

- flow of air around supersonic aircraft
- shock waves! (nonlinear effect)
- aerospace engineers were the first to develop numerical methods for the Euler equations
Application 2: Supersonic Solar Wind Physics

- heat from sun core accelerates radial flow from subsonic to supersonic
- bow shock at the earth!
Application 3: Sedimentation in Mechanical Engineering
Time for some reflection...

• 3 different applications, same mathematics!

• “power of mathematical abstraction”

• driving force of the computational and applied mathematician!
Application 4: 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
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
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!
transonic radial outflow solution

subsonic $\Rightarrow|\Leftarrow$ supersonic
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:**
  - mass flux (mass/time) (how fast does the planet evaporate?)
  - location of critical point
numerical method

- 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
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

\[
\frac{U_{i}^{n+1} - U_{i}^{n}}{\Delta t} + \frac{F_{i+1/2} - F_{i-1/2}}{\Delta r} = S(U_{i})
\]

• CM452: Numerical Partial Differential Equations
• very slow convergence to steady state... (more later!)
Simulations of planet atmosphere
results for 1D exoplanet simulations

• HD209458b:
  - lower boundary conditions $\rho = 7.10^{-9}$ g/cm$^3$ and $T=750$K
  - extent of atmosphere, outflow velocity, and mass flux consistent with observations (Vidal-Madjar 2003)
  - 1% mass loss in 12 billion years $\implies$ HD209458b is stable

• Tian, Toon, Pavlov, and De Sterck, Astrophysical Journal 621, 1049-1060, 2005
2D numerical models (Scott Rostrup, NSERC USRA summer 2005, and now Master’s)

- Euler equations in multiple dimensions

\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \vec{v} \\ \frac{p}{\gamma - 1} + \frac{\rho v^2}{2} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \vec{v} \\ \rho \vec{v} \cdot \vec{v} + I p \\ \frac{\gamma p}{\gamma - 1} + \frac{\rho v^2}{2} \end{bmatrix} = \begin{bmatrix} 0 \\ \vec{F}_{ext} \\ \vec{F}_{ext} \cdot \vec{v} + q_{heat} \end{bmatrix}
\]
2D Simulations

• assume rotational symmetry about the y axis

⇒ allows for non-uniform heating
non-uniform heating

- heated by a thin layer in the northern hemisphere
- outflow mass flux similar to 1D case
- 1D gives reasonable approximation
ongoing work: include stellar wind
3D numerical models (Paul Ullrich, NSERC USRA summer 2005, now Master’s)

- we want to include effects of planetary rotation
Some more reflection now...

What is computational mathematics? (my take...)

1) apply existing mathematical methods to solve problems on computers
   - science, engineering, finance, health, internet, technology, ....

2) develop new mathematical methods to solve problems faster, more accurately, more reliably
   - can be very theoretical! (convergence or complexity proofs, ...)

⇒ both in close collaboration with application specialists!
2) Can we solve the steady Euler equations faster and more accurately?

- Yes!

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

- New approach: solve the steady equations directly

\[
\frac{dF(U)}{dr} = S(U)
\]

\[
\frac{d}{dr} \begin{bmatrix}
\rho \frac{u r^2}{u^2} \\
\rho u^2 r^2 + p r^2 \\
\gamma p \left( \frac{1}{\gamma - 1} + \frac{\rho u^2}{2} \right) u r^2 \\
\end{bmatrix}
= \begin{bmatrix}
0 \\
-\rho G M + 2 p r \\
-\rho G M u + q_{\text{heat}} r^2 \\
\end{bmatrix}
\]
Solving the steady ODE system is hard...

- consider toy problem (simplified): single ODE

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

- normally need 1 boundary condition to determine solution
- transonic solution: no boundary condition needed!
Solving the steady ODE system is hard...

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

- but... integrating outward from the critical point does work!!!
Direct calculation of steady solution

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

1. Write as dynamical system...

\[
\frac{du(s)}{ds} = -2u c^2 \left( r - \frac{GM}{2c^2} \right) \quad \frac{dV}{ds} = G(V)
\]

\[
\frac{dr(s)}{ds} = -r^2 (u^2 - c^2)
\]

2. find critical point: \( G(V) = 0 \)

3. linearize about critical point

\[
\frac{\partial G}{\partial V} \bigg|_{V_{crit}} = \begin{bmatrix} 0 & 2c^3 \\ \frac{(GM)^2}{2c^3} & 0 \end{bmatrix}
\]

4. integrate outward from critical point
For the Full Euler Equations

\[
\frac{d}{dr} \begin{bmatrix}
\rho u r^2 \\
\rho u^2 r^2 + p r^2 \\
(\frac{\gamma p}{\gamma-1} + \frac{\rho u^2}{2}) u r^2
\end{bmatrix} = \begin{bmatrix}
0 \\
-\rho GM + 2 pr \\
-\rho GM u + q_{\text{heat}} r^2
\end{bmatrix}
\]

• problem: there are many possible critical points!
New algorithm for calculating steady transonic Euler outflows

1. Use adaptive ODE integrator to find trajectory
2. Modify guess for critical point depending on deviation from desired inflow boundary conditions (Newton method)
3. Repeat
New algorithm for calculating steady transonic Euler outflows

new algorithm:
• much faster than time marching
• much more accurate (adaptive RK45)
• CM352: Numerical Ordinary Differential Equations

⇒ Computational Mathematics research finds new, better methods to solve problems on computers
Application 5: 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
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 ⇒ 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
Lessons learned...

Computational mathematics is...

1) apply existing mathematical methods to solve problems on computers

2) develop new mathematical methods to solve problems faster, more accurately, more reliably

⇒ both in close collaboration with application specialists!
We need bright students to help in research...

1) NSERC undergraduate student research award program (4 months in summer)

2) Waterloo’s brand new one-year Master’s program in Computational Mathematics (broad introduction to a variety of Computational Mathematics areas, starts September 2008)

3) Master’s and PhD in Computational Mathematics-related research areas at Waterloo’s Math faculty
• Questions?
Supersonic gas escape from Early Earth

- there is no supersonic hydrodynamic escape from present-day Earth
- exo-base temperature is high: collisional, thermal escape dominates
Supersonic gas escape from Early Earth

- hypothesis: when the Earth was young, the exo-base temperature may have been low, and supersonic hydrodynamic escape may have been ongoing
- test of hypothesis: do 1D simulation, find exobase temperature, and outflow flux

⇒ our simulations confirm cold exobase and hydrodynamic escape with small mass flux

this finding also has implications for hydrogen content in Early Earth atmosphere!
Lessons learned...

Computational mathematics is cool!

CM undergraduate program:
(http://www.math.uwaterloo.ca/navigation/CompMath)

  choose 2 out of our 5 streams: differential equations, linear algebra, discrete math, optimization, statistics

  or choose one of our 4 new options:
  1) biomedical
  2) earth and space
  3) data mining
  4) economics
Application 3: Sedimentation in Mechanical Engineering

Strong lines are the predictions and paler lines the corresponding measured porosities. Numbers mark the elapsed time in minutes.

Predicted porosity profile at 399 minutes. There is no corresponding measurement.
transonic radial outflow solution: problem definition

- Euler equations: 3 equations in three variables
  \[ \rho(r, t), u(r, t), p(r, t) \]
- lower boundary at planet surface: subsonic, needs two boundary conditions: density and pressure
- upper boundary: supersonic, needs no boundary conditions (all information flows out)