Numerical simulations of fluid models in astrophysics
From stellar jets to CO white dwarfs
(or, how things sometimes work pretty well and sometimes do not)

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Many astrophysical phenomena, that range from super-sonic flows from proto-stars to novae explosions can be described by hydro-dynamic or magneto-hydrodynamic fluid equations.

Despite their basic simplicity, solving these equations via numerical calculations is still a big challenge, because of the wide range of scales, and/or the stiff source terms in the energy equation.

Achieving reliable results is not a trivial matter. Reliability is a complicate function of both numerical (resolution, scheme order) and physical parameters.

The next two examples show how numerical viscosity, in particular, may dramatically affect the results.
Bright knot formation in HH objects
Supersonic flows from young stars have been widely imaged in the recent past by the Hubble telescope, and details of the morphology, kinetic and emission properties of the so-called ‘optical knots’ are now available.

Question: what is the origin of the knots? Why do they move?

Recent observations of HH-111 show that the emissivity [SII] and H$_\alpha$ intensity decay, respectively, as $L^{-1.9}$ and $L^{-2.4}$, suggesting that in the absence of recombination effects during the jet lifetime (too short with respect to the recombination time scale), such decay is probably due to the opening angle and the corresponding volume growth, that would make density decay as $L^{-2}$. 

![Graph showing [SII] and H$_\alpha$ intensity over time](image)
We claim that internal shocks (IS) can play some role in the formation of moving bright knots.

Objections

a) IS are smoothed away in cooling jets by radiative losses;
b) IS pattern is stationary → the need of ‘pulsating inflow conditions’.

Our answers

a) IS survival mostly depends on the density ratio (Blondin 1992);
b) steady patterns strictly apply to steady b.c. only;
The non-equilibrium model in the numerical code

Euler HD eqs. + electrons + H2 conservation equations, including atomic hydrogen (H) ion/rec and molecular hydrogen (H2) dissociation. Metals with solar abundances and constant mass fraction have also been considered; Cooling losses from H and H2 also below $10^4$ K;

Input simulation parameters

density ratio $D_r$, pressure ratio $P_r$, e and H2 initial densities, inflow velocity, nozzle radius $r_{jet}$;

Diagnostics

SII, Ha emissivity maps, X and radio maps et al.;
Initial parameters setup

$T_{\text{jet}} = 6000 \text{ K} \quad (\text{Bacciotti 1997}); \quad T_{\text{ISM}} = 100 \text{ K} \quad (\text{unpert. ISM})$

$N_{e_{\text{jet}}} = 0.3 \quad N_{\text{H}_2_{\text{ISM}}} = 0.5 \quad \text{(particle fractions)}$

$V_{\text{jet}} = 200 \text{ Km/s} \rightarrow \text{Mach number} \sim 20$

$r_{\text{jet}} = 0.5 \times 10^{15} \text{ cm} \rightarrow \frac{dM}{dt} = 5 \times 10^{-8} \text{ SM/yr}$

$P_{r} = 600 \rightarrow 6, \quad D_{r} = [10, 0.1] \rightarrow \text{under-expanded, light jets}$

In which range of $P_{r}$ and $D_{r}$ do IS form?
Under-expanded, heavy jets

$P_r = 600$, $D_r = 10$

No IS!
The pressure ratio must be lowered as much as possible in order to form IS on the jet length scale. This creates

under-expanded, light jets

\[ P_r = 6, \ D_r = 0.1 \]

a) log density map
b) log SII emission map
c) integrated SII map
What about the influence of the nozzle radius on the knots pattern?

$P_r = 6$, $D_r = 0.4$

$r_{\text{jet}} = 10^{14}$ cm

under-expanded, small radius, light jets

a) log density map

b) log SII emissivity map

c) integrated SII map
Same parameters as the previous jet example. The flow has been switched-off, then restored 100 years later. From top to bottom and left to right, shots at \( t = 800, 850, 900, 950, 1000, 1050, 1100 \) and 1200 yr.
The good guy.

In this problem, the numerical simulations yield a good reproduction of the astrophysical object. They also succeed at verifying the hypothesis about the role of the IS, and provide the range of the flow parameters. The results are proven to be “resolution convergent”
Hydrogen from the companion star piles up in the C-O white dwarf (WD) atmosphere. Density, pressure and temperature grow at the bottom of the atmosphere. Heavy metals from the star are dredged-up and mixed with the atmospheric gas.

When $T$ approaches $1.0 \times 10^8$ K thermo-nuclear reactions (TNR) become more and more efficient, and $T$ grows faster and faster. At $T = 2.0 \times 10^8$ K the runaway takes place, and metals are ejected.
Numerical simulation: from the initial conditions to the runaway

1) 1D equilibrium models are given, that provide P, ρ, T and species mass fractions as a function of the atmosphere height.

2) The equilibrium fields are projected onto the 2D code mesh.

3) The initial equilibrium is perturbed, linear instabilities grow and eventually saturate.

4) Thermonuclear reactions are switched on, together with the network transport equations and the system evolves toward the runaway.
FAQ:

1) What is the mechanism (gravity waves? K-H instabilities? convective motions?) that lifts up C, O and other metals from the core into the envelope?

2) How does the runaway take place?

3) How much of matter can be dredged-up?

This is an initial condition, stability problem. We can show that questions # 1 and # 2 can be addressed numerically, whereas “quantitative” questions such as # 3 are still far from answerable given our current calculation capabilities.
1D equilibrium initial conditions

Below from top/left, clockwise: density, pressure, temperature and some species mass fractions vs. r (in cgs units)
From the literature (2-nd order, ideal simulations)

- From $t=0$ to $t \approx 150$ seconds: weak convective instabilities move some C-O from the core as the burning rate grows steadily. At $t=240$ s is $T \approx 2 \times 10^8$ K, the energy is no longer transported by convection and the runaway takes place.

Luminosity (left) and horizontally averaged T profile from i.c. to the run-away (right)

The aforementioned results show weak and laminar convective motions and very poor mixing. In our opinion they are strongly affected by the code numerical viscosity and **numerical Rayleigh number**, ($Ra_{\text{num}} \sim$ a few $10^4$).
In order to perform less viscous simulations of the pre-runaway burning convection a new code has been developed at the ASC Flash Center of the University of Chicago and at the Dept. of Astronomy of the University of Florence. CONVAIR is a parallel, high order, low numerical viscosity code, suited for subsonic or shock-free supersonic flows.

**Numerical features**

- Cartesian geometry, non-uniform mesh in the radial direction.
- Fourier/Compact differences transforms in the horizontal/radial direction.
- Explicit/semi-implicit time-advancing scheme --> affordable long-time simulations by skipping the CFL constraint from sound waves and viscous term.

**and physical models from the FLASH code**

- Euler/Navier Stokes equations + 12 transport equations for the species involved in TNR (CNO cycle). At each time-step the network updates the mass fractions and the nuclear reaction energy source term.

- Ideal equation of state (EOS) and/or Helmoltz EOS for degenerate gas (Timmes et al., ApJ SS, 125,1999).
Simulation # 1
Non-ideal model, $\kappa = \kappa_{\text{real}} \times 10^5$, $\nu$ such that $t_\nu = t_\kappa$
$Ra \sim 20000$ (as in the literature)
Simplified model for TNR energy generation, $E \sim \rho [H]^2 T^{18}$;
The velocity field in the convective region allows an estimate of the turbulent diffusion time scale.

Dynamics at $t= 300s$.

Left: velocity field from $5.4 \times 10^3$ to $5.7 \times 10^3$ Km, close to the temperature peak.

Right: density field. Small scale rolls form, with show $d \sim 30$ Km (3 grid zones).
**Turbulent diffusion time scale**:

Assuming fully developed turbulence, the turbulent diffusion coefficient for a scale $L$ is $D_L \sim a V L$, with $a = 0.1$ (Young, 1989). In our simulation we observe $L_{\text{min}} \sim 3 \times 10^6$ cm, $V \sim 5 \times 10^7$ cm/s $\Rightarrow D_L \sim 1.5 \times 10^{14}$ cm$^2$/s $\Rightarrow$

$$t_{TD} \sim \frac{L^2}{D_L} \sim 6 \times 10^{-2} \text{ s}$$

**Burning time scale**:

According to the simplified model for TNR heat generation, $E \sim \rho H^2 T^{18}$, $t_{TNR} \sim \frac{1}{(\rho H^2 T^{17})} \Rightarrow$

$$t_{TNR_{\text{min}}} > 10 \text{ s as long as } T_{\text{max}} \sim 1 \times 10^8 \text{ K}$$

**Scenario**

As long as $t_{TD} < t_{TNR}$ (turbulence driven regime, from $t=0$ to $t\sim 300$ s) the energy released by TNR is expected to diffuse, heating the gas above and overheating the gas laterally. In this regime temperature fluctuations are equalized by turbulent motions.

As the average value of $T$ increases, hot spots can randomly form, in which the condition $t_{TD} > t_{TNR}$ (burning regime) is locally satisfied, TNR are self-sustained and the gas evolves toward the runaway.
Horizontally averaged temperature profile
Temperature field
**Turbulence driven phase**: $t_{DT} \sim 6 \times 10^{-2}$ s, $t_{TNR} \sim 1000$ s ($T_{av} \sim 80$ MK)

- $T=387$ s
- $T=387.75$ s
- $T=388.5$ s

**TNR driven phase**: $t_{DT} \sim 6 \times 10^{-2}$ s, $t_{TNR} \sim 10^{-5}$ s ($T_{av} \sim 110$ MK)

- $T=572.71$ s
- $T=572.75$ s
- $T=572.76$ s
The runaway
Density profile: at $t=0$ (solid line) and at $t=600$ s (dotted line)

At $t = 600$ s the density profile shows some change with respect to the initial value.
If $\nu$ and $\kappa$ are large enough to lower the initial Rayleigh number, a “controlled” burning convection process occurs in the pre-runaway phase.

As long as $8 \times 10^7 \text{ K} < T < 1 \times 10^8 \text{ K}$

temperature fluctuations are equalized by the turbulent diffusion and $T$ increases uniformly.

When and where $T > 1 \times 10^8 \text{ K}$

TNR dominate. Temperature fluctuations drive the formation of self-sustained hot spots with $T$ as high as $2 \times 10^8 \text{ K}$.

Next steps

Use larger and larger Rayleigh numbers, measure the horizontally averaged kinetic energy spectra and the mixing effects and look for asymptotic behavior with $R_a$. 
Simulation # 2:
Ideals model $\Rightarrow \nu = 0, \kappa = 0$

$$Ra = \varepsilon L^3 g / (\nu \kappa) = Ra_{\text{num}} \sim 80000$$

velocity pattern
temperature field
Conclusions

Numerical simulations of systems with equilibrium initial conditions often yield more challenging problems than non-equilibrium systems, since instabilities develop according to the value of some “characteristic number” that depends on the physical parameters.

In most astrophysical applications the parameters are such that these numbers largely exceed our computations capabilities. In these cases care must be taken when running ‘ideal models’, in which physical parameters and characteristic numbers are determined by the numerical viscosity of the code.

As in the white-dwarf problem, it happens to put together a bad physical model (initial conditions) and a bad numerical tool (2-nd order scheme) to catch “good results”. A systematic procedure for numerical experiments would show that, unfortunately, they do not converge with numerical and physical parameters.

A systematic procedure requires that realistic non-dimensional parameters be used in the equations and the “correct” solution determined via asymptotic extrapolation of the numerical results.

So, watch the step!