WENO 3D Numerical Simulation of High Mach Number Astrophysical Jets

Carl Gardner & Jeremiah Jones
Arizona State University
Herman Melville: *not only ubiquitous, but immortal (for immortality is but ubiquity in time)*
Chandra/ESO/VLA Image of Centaurus A Jets, 
\(d = 12\) Mly, \(l_j = 100\) kly
Hubble Image of Carina Nebula, $d = 10$ kly, $l_j = \frac{1}{2}$ ly
Hubble Image of HH 47 Jet, $d = 1500$ ly, $l_j = \frac{1}{2}$ ly
Hubble Image of HH 24 Jets, $d = 1350$ ly, $l_j = \frac{1}{2}$ ly
Gas Dynamics with Radiative Cooling

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0, \quad \rho = mn \]

\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_i} (\rho u_i u_j + P \delta_{ij}) = 0 \]

\[ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i} (u_i (E + P)) = -C(n, T) \]

with pressure given by polytropic gas equation of state \((\gamma = 5/3)\)

\[ P = (\gamma - 1) \left( E - \frac{1}{2} \rho u^2 \right) = nk_B T \]

Without radiative cooling, similarity transformation \(x_i \rightarrow ax_i, t \rightarrow at\)
leaves gas dynamical equations invariant
Radiative Cooling Function

\[
C(n, T) = \begin{cases} 
  n^2 \Lambda(T) & T \geq 8000 \text{ K}, \text{ atomic cooling only} \\
  nW(n, T) & 100 \text{ K} \leq T < 8000 \text{ K}, \text{ H}_2 \text{ cooling only}
\end{cases}
\]

Atomic cooling (Schmutzler & Tscharnuter) includes relevant emission lines of 10 most abundant elements \( \text{H, He, C, N, O, Ne, Mg, Si, S, Fe} \) in interstellar medium + relevant continuum processes

Molecular cooling from Le Bourlot, Pineau des Forêts, & Flower

In \( n \) above 8000 K, H comprises 91%, He 9%, & “metals” 0.1%

For \( T < 8000 \text{ K}, \text{ H} \rightarrow \text{ H}_2 \)
Radiative Cooling Function $\Lambda = C/n^2$
Numerical Methods

- 3D WENO code for non-relativistic gas dynamics with radiative cooling

- Third- & fifth-order WENO in space, third-order RK in time

- Parallelized with OpenMP & MPI
Parallelization with Domain Decomposition

- MPI (Message Passing Interface) is used to distribute 3D domain across multiple computing nodes

- Each node exchanges boundary data with nodes corresponding to neighboring subgrids

- OpenMP threading is used to employ all cores on a node

- Computations for each dimension by dimension WENO sweep are completely decoupled & ideal for threading
Third-Order WENO Scheme

1D scalar conservation law

\[ q_t + f(q)_x = 0, \quad \partial f(q)/\partial q \geq 0 \]

WENO (Liu, Osher, & Chan; Jiang & Shu) uses a convex combination of all candidate stencils:

\[
\frac{dq_j(t)}{dt} + \frac{1}{\Delta x} \left( F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} \right) = 0
\]

\[
F_{j+\frac{1}{2}} = \omega_1 F_{j+\frac{1}{2}}^{(1)} + \omega_2 F_{j+\frac{1}{2}}^{(2)}
\]

\[
F_{j+\frac{1}{2}}^{(1)} = -\frac{1}{2}f_{j-1} + \frac{3}{2}f_j, \quad F_{j+\frac{1}{2}}^{(2)} = \frac{1}{2}f_j + \frac{1}{2}f_{j+1}
\]

\[
F_{j-\frac{1}{2}}^{(1)} = -\frac{1}{2}f_{j-2} + \frac{3}{2}f_{j-1}, \quad F_{j-\frac{1}{2}}^{(2)} = \frac{1}{2}f_{j-1} + \frac{1}{2}f_j
\]
Third-Order WENO Stencil near a Shock Wave

\[
q_t + f(q)_x = 0, \quad \partial f / \partial q \geq 0
\]

\[
\frac{dq_j}{dt} + \frac{1}{\Delta x} \left( F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} \right) = 0, \quad F_{j-\frac{1}{2}}^{(1)} \text{ suppressed}
\]
Third-Order WENO Scheme

Nonlinear weights

\[ \omega_m = \frac{\tilde{\omega}_m}{\sum_{l=1}^{2} \tilde{\omega}_l}, \quad \tilde{\omega}_l = \frac{\gamma_l}{(\varepsilon + \beta_l)^2}, \quad \varepsilon = 10^{-6} \]

where linear weights \( \gamma_1 = \frac{1}{3}, \quad \gamma_2 = \frac{2}{3} \) & smoothness indicators \( \beta_1 = (f_j - f_{j-1})^2, \quad \beta_2 = (f_{j+1} - f_j)^2 \)

If \( \partial f(q)/\partial q \) changes sign, use Lax-Friedrichs flux splitting

\[ f(q) = f^+(q) + f^-(q) \]

\[ f^\pm(q) = \frac{1}{2} (f(q) \pm \alpha q), \quad \alpha = \max_q |\partial f(q)/\partial q| \]

For gas dynamics, \( \alpha = \max\{|u| + c_s\} \)
WENO Scheme

For hyperbolic systems, apply WENO in local characteristic fields:
\[ w = Rq, \; R = \text{Roe matrix} \]

For 2D & 3D, apply WENO in each spatial direction (dimension by dimension splitting)

Time discretization: third-order TVD Runge-Kutta method

\[
q^{(1)} = q^n + \Delta t L(q^n, t_n)
\]
\[
q^{(2)} = \frac{3}{4} q^n + \frac{1}{4} q^{(1)} + \frac{1}{4} \Delta t L(q^{(1)}, t_n + \Delta t)
\]
\[
q^{n+1} = \frac{1}{3} q^n + \frac{2}{3} q^{(2)} + \frac{2}{3} \Delta t L(q^{(2)}, t_n + \Delta t/2)
\]

where \( L(q, t) \approx -\partial f(q)/\partial x \)
WENO Scheme

For stability

$$\alpha \frac{\Delta t}{\Delta x} \leq 1$$

where $\alpha = \max\{|\lambda| \frac{\partial f}{\partial q}\} = \max\{|u| + c_s\}$ (gas dynamics)

Cooling term

$$\frac{\partial E}{\partial t} + \cdots = -C(n, T)$$

is incorporated within RK3 solver
Positivity Preserving WENO Scheme

Flux limiter to guarantee $\rho > 0$ & $P > 0$ for homogeneous gas dynamics:

$$F_{j + \frac{1}{2}} = \left(1 - \theta_{j + \frac{1}{2}}\right) F_{j + \frac{1}{2}}^{LF} + \theta_{j + \frac{1}{2}} F_{j + \frac{1}{2}}^{WENO}$$

where $0 < \theta_{j + \frac{1}{2}} \leq 1$ is chosen by positivity preserving algorithm of Hu, Adams, & Shu, with

$$\alpha \frac{\Delta t}{\Delta x} < \frac{1}{2}$$

Can also insure that source term ODE contribution is positivity preserving
SVS 13 Jet & Bow Shock Bubble

with Klaus Hodapp (Hawaii)
Keck Image of SVS 13, $d = 750$ ly, $l_j = 4$ ldy
**SVS 13 Jet Parameters**

<table>
<thead>
<tr>
<th>jet</th>
<th>ambient</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_j = 1000 \text{ H/cm}^3$</td>
<td>$n_a = 1000 \text{ H}_2/\text{cm}^3$</td>
</tr>
<tr>
<td>$u_j = 156 \text{ km/s}$</td>
<td>$u_a = 0$</td>
</tr>
<tr>
<td>$T_j = 1000 \text{ K}$</td>
<td>$T_a = 500 \text{ K}$</td>
</tr>
<tr>
<td>$c_{s,j} = 3.7 \text{ km/s}$</td>
<td>$c_{s,a} = 2.6 \text{ km/s}$</td>
</tr>
<tr>
<td>$M_{j,j} = 40$</td>
<td>$M_{j,a} = 60$</td>
</tr>
</tbody>
</table>

Cyl Sym: $1200 \Delta z \times 400 \Delta r$, $(3.3, 2.2) \times 10^{10} \text{ km}$

3D: $500 \Delta x \times 500 \Delta y \times 500 \Delta z$, $2 \times 10^{10} \text{ km on a side}$

$\bar{n} = 100 \text{ H/cm}^3$

$\bar{T} = 10,000 \text{ K}$
SVS 13 Bow Shock Bubble at 18.5 Yr
Mach 60 SVS 13 Jet & Bow Shock Bubble at 20.4 Yr
SVS 13 Jet & Bow Shock Bubble at 21.1 Yr
SVS 13 Jet & Bow Shock Bubble at 22.3 Yr
SVS 13 Jet & Bow Shock Bubble Bubble at 26.1 Yr
SVS 13 Jet & Bow Shock Bubble at 30 Yr
Keck Image of SVS 13, $d = 750$ ly, $l_j = 4$ ldy
Asymmetric SVS 13 Jet & Bow Shock Bubble at 21 Yr
HH 30 Jet near Its Launch Site, $d = 450$ ly, $l_j = 3.5$ ldy

with Perry Vargas (ASU), Hubble images by Hartigan & Morse

Fig. 10.—Same as Fig. 9, but for the electron temperature, electron density, and hydrogen ionization fraction $X_H = H^+/(H + H^+)$). The area of high excitation (high $X_H$ and $T_e$, color-coded as yellow and white) in knot B moves outward with the flow. The jet emerges with a very low ($\leq 0.1$) ionization fraction and becomes more ionized beyond $\sim 50$ AU. At large distances the ionization declines.
HH 30 Jet Parameters

<table>
<thead>
<tr>
<th>jet</th>
<th>ambient</th>
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</thead>
<tbody>
<tr>
<td>$n_j = 10^5$ H/cm³</td>
<td>$n_a = 2.5 \times 10^4$ H₂/cm³</td>
</tr>
<tr>
<td>$u_j = 300$ km s⁻¹</td>
<td>$u_a = 0$</td>
</tr>
<tr>
<td>$T_j = 10^4$ K</td>
<td>$T_a = 10^3$ K</td>
</tr>
</tbody>
</table>

Cyl Sym: $750\Delta z \times 100\Delta r$, $(1.5, 0.4) \times 10^{11}$ km
Jet periodically pulsed: on for 6.5 yr & off for 1.5 yr over 35 yr
Mach 25 HH 30 Jet: HST to $0.94 \times 10^{11}$ km
HH 30 Jet: HST to $0.94 \times 10^{11}$ km
HH 30 Jet

Blue curves from Hartigan & Morse, cyan by Tesileanu et al.
HH 30 Jet

[N II] Surface Brightness

\[ \log_{10}(S) \]

arcsec

-18
-17
-16
-15
-14
-13
-12

[N II] obs
[N II] T sim
[N II] our sim
HH 30 Jet

[S II] Surface Brightness

$\log_{10}(S)$ vs arcsec

- [S II] obs
- [S II] T sim
- [S II] our sim
HH 30 Jet: $t_{\text{equil}}/t_{\text{cool}}$, $t_{\text{equil}} \approx t_{\text{rec}}$ for $\text{H}^+ + e^- \rightarrow \text{H} + \gamma$
Centaurus A Jet & Star Formation, $d = 12$ Mly, $l_j = 100$ kly

with Evan Scannapieco & Rogier Windhorst (ASU)
Image by Chandra/ESO/VLA
Chandra Image of Cen A Jets
Chandra/ESO/VLA Image of Cen A Jets
Hubble Image of Star Forming Regions near Cen A Jet

Located 30 kly from nucleus & 7.5 kly away from jet
Hubble Closeup of Region 1 near Cen A Jet
Star Formation by AGN Jet

Cen & Ostriker (1992)

(i) \( \nabla \cdot \mathbf{u} < 0 \) (true for bow shock compression)

(ii) \( t_{cool} = E/|dE/dt| \ll t_{grav} \sim 1/\sqrt{G\rho} \sim 10 \text{ Myr} \)

(iii) Jeans unstable: \( M_{cloud} > M_{Jeans} = G^{-3/2} \rho^{-1/2} c_s^3 \)
**Cen A Jet, Ambient, & Cloud Parameters**

<table>
<thead>
<tr>
<th>jet</th>
<th>ambient</th>
<th>clouds</th>
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</thead>
<tbody>
<tr>
<td>$n_j = 0.01$ H/cm$^3$</td>
<td>$n_a = [0.02,0.2]$ H/cm$^3$</td>
<td>$n_c = [2,75]$ H$_2$/cm$^3$</td>
</tr>
<tr>
<td>$u_j = 4 \times 10^4$ km/s</td>
<td>$u_a = 0$</td>
<td>$u_c = 0$</td>
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$420\Delta x \times 420\Delta y \times 420\Delta z$, 6300 ly on a side

$u_{prop} = 1.2 \times 10^4$ km/s, Mach number 1000

$D_{cloud} = [425,1050]$ ly, $M_{cloud} = [0.2, 3.4] \times 10^6 M_\odot$

$D_{cluster} = 80$ ly, $M_{cluster} = [1,2] \times 10^4 M_\odot$

3D computations took 100,000 CPU hours (11.5 CPU years!)

SDSC Comet XSEDE computer cluster using 1200 cores

Wall time: 130 hours (5.4 days) = 65% efficiency
3D Simulation of Cen A Jet: Initial Conditions
Mach 1000 Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Cen A Jet at 780,000 yr
Star Formation
Star Clusters Formed at 780,000 yr

<table>
<thead>
<tr>
<th>cloud</th>
<th>(n_{\text{max}})</th>
<th>(D_{\text{cloud}}/\text{pc})</th>
<th>(M_{\text{cloud}}/(10^5 , M_\odot))</th>
<th>(t_f)</th>
<th>(N_{20\text{pc}})</th>
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</table>
Cen A Jet at 3 Myr $\approx t_{\text{grav}}/3$