Non-equilibrium Chemistry with the FLASH Code

Kyujin Kwak

Ulsan National Institute of Science and Technology (UNIST)

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Non-Equilibrium Ionization Calculation with FLASH

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) + \nabla P &= \rho \mathbf{g} \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[(\rho E + P)\, \mathbf{v} \right] &= \rho \mathbf{v} \cdot \mathbf{g} \ \left[+ S \right] \\
\frac{\partial n_i^Z}{\partial t} + \nabla \cdot n_i^Z \mathbf{v} &= R_i^Z \quad (i = 1, \ldots, N_{spec}) \ ,
\end{aligned}
$$

$$
R_i^Z = N_e [n_{i+1}^Z \alpha_{i+1}^Z + n_{i-1}^Z S_{i-1}^Z - n_i^Z (\alpha_i^Z + S_i^Z)] \ ,
$$

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FORMATION OF COMPACT STELLAR CLUSTERS BY HIGH-REDSHIFT GALAXY OUTFLOWS. I. NON-EQUILIBRIUM COOLANT FORMATION

William J. Gray and Evan Scannapieco
School of Earth and Space Exploration, Arizona State University, P.O. Box 871404, Tempe, AZ 85287-1404, USA

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ABSTRACT

We use high-resolution three-dimensional adaptive mesh refinement simulations to investigate the interaction of high-redshift galaxy outflows with low-mass virialized clouds of primordial composition. While atomic cooling allows star formation in objects with virial temperatures above 10^4 K, "minihalos" below this threshold are generally unable to form stars by themselves. However, these objects are highly susceptible to triggered star formation, induced by outflows from neighboring high-redshift starburst galaxies. Here, we conduct a study of these interactions, focusing on cooling through non-equilibrium molecular hydrogen (H_2) and hydrogen deuteride (HD) formation. Tracking the non-equilibrium chemistry and cooling of 14 species and including the presence of a dissociating background, we show that shock interactions can transform minihalos into extremely compact clusters of coeval stars. Furthermore, these clusters are all less than $\approx 10^6\ M_\odot$, and they are ejected from their parent dark matter halos: properties that are remarkably similar to those of the old population of globular clusters.

Key words: astrochemistry – galaxies: formation – galaxies: high-redshift – galaxies: star clusters: general – globular clusters: general – shock waves

Online-only material: color figures

Reactors and Reaction Networks

- Atomic hydrogen (H, H^+, H^-) : A=1
- Atomic deuterium (D, D^+, D^-) : A=2
- Atomic helium (He, He^+, He^{++}) : A=4
- Molecular hydrogen (only two states: H_2, H_2^+) : A=2
- Molecular hydrogen deuteride (only two states: HD, HD^+): A=3
- Total 13 species + electrons
- 84 reactions
- From Glover & Abel 2008

Reaction Calculation

$$X_i \equiv \rho_i/\rho = n_i A_i/(\rho N_A), \quad N_A = \frac{1}{m_A} \tag{1}$$

$$Y_i \equiv X_i/A_i = n_i/(\rho N_A), \tag{2}$$

$$\dot{Y}_i \equiv \frac{dY_i}{dt} = \dot{R}_i, \tag{3}$$

$$i + j \rightarrow k + l,$$

$$\dot{R}_i \equiv \sum_{j,k} Y_l Y_k \lambda_{\mathrm{kj}}(l) - Y_i Y_j \lambda_{\mathrm{jk}}(i), \tag{4}$$

Reaction Calculation (Cont'd)

$$\dot{R}_i \equiv \sum_{j,k} Y_l Y_k \lambda_{\rm kj}(l) - Y_i Y_j \lambda_{\rm jk}(i) - Y_i J(\nu_\alpha), \qquad (5)$$

the background radiation, $J(\nu_\alpha)$.

$$Y_{\rm elec} = Y_{\rm H^+} + Y_{\rm D^+} + Y_{\rm HD^+} + Y_{\rm H_2^+} + Y_{\rm He^+} + 2Y_{\rm He^{++}} - Y_{\rm H^-} - Y_{\rm D^-}. \quad (6)$$

Non-Equilibrium Ionization Calculation with FLASH

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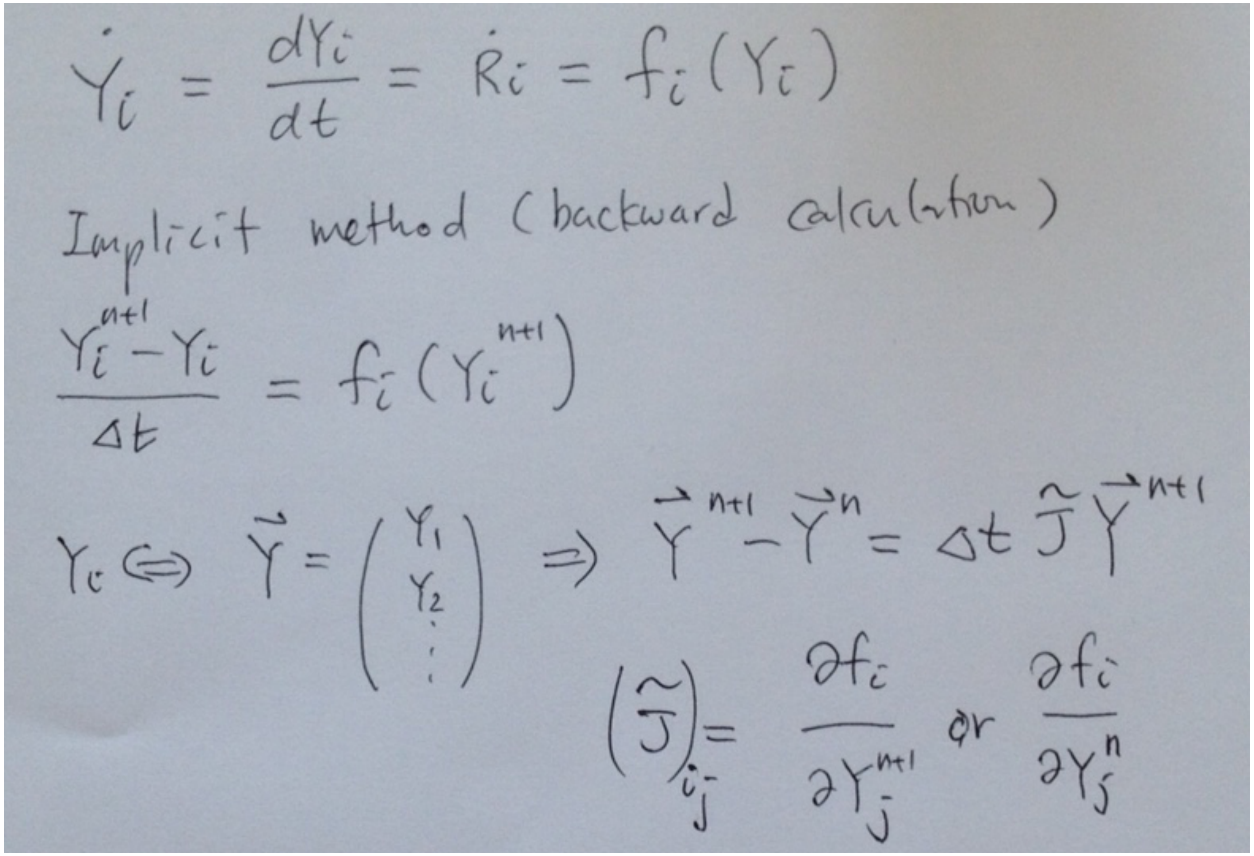
R_i^Z = N_e [n_{i+1}^Z \alpha_{i+1}^Z + n_{i-1}^Z S_{i-1}^Z - n_i^Z (\alpha_i^Z + S_i^Z)] \ ,
$$

Reaction Calculation (Cont'd)



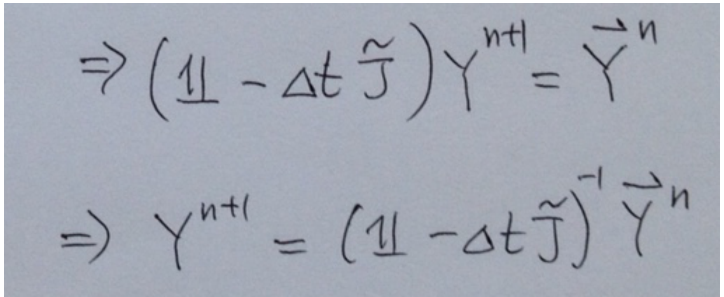
$$\dot{Y}_i = \frac{dY_i}{dt} = \dot{R}_i = f_i(Y_i)$$

Implicit method (backward calculation)

$$\frac{Y_i^{n+1} - Y_i}{\Delta t} = f_i(Y_i^{n+1})$$

$$Y_i \Leftrightarrow \vec{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \end{pmatrix} \Rightarrow \vec{Y}^{n+1} - \vec{Y}^{n} = \Delta t \, \tilde{J} \, \vec{Y}^{n+1}$$

$$(\tilde{J})_{ij} = \frac{\partial f_i}{\partial Y_j^{n+1}} \text{ or } \frac{\partial f_i}{\partial Y_j^{n}}$$



$$\Rightarrow (\mathbb{1} - \Delta t \, \tilde{J}) Y^{n+1} = \vec{Y}^{n}$$

$$\Rightarrow Y^{n+1} = (\mathbb{1} - \Delta t \, \tilde{J})^{-1} \vec{Y}^{n}$$

Reaction Calculation (Cont'd)

$$\mathbf{Y}^{n+1} = \mathbf{Y}^n + \sum_{i=1}^{4} b_i \boldsymbol{\Delta}_i, \tag{7}$$

$$(\hat{1}/\gamma h - \bar{J}) \cdot \boldsymbol{\Delta}_1 = f(\mathbf{Y}^n), \tag{8}$$

$$(\hat{1}/\gamma h - \bar{J}) \cdot \boldsymbol{\Delta}_2 = f(\mathbf{Y}^n + a_{21}\boldsymbol{\Delta}_1) + c_{21}\boldsymbol{\Delta}_1/h, \tag{9}$$

$$(\hat{1}/\gamma h - \bar{J}) \cdot \boldsymbol{\Delta}_3 = f(\mathbf{Y}^n + a_{31}\boldsymbol{\Delta}_1 + a_{32}\boldsymbol{\Delta}_2) + (c_{31}\boldsymbol{\Delta}_1 + c_{32}\boldsymbol{\Delta}_2)/h, \tag{10}$$

$$\begin{aligned}(\hat{1}/\gamma h - \bar{J}) \cdot \boldsymbol{\Delta}_4 = {} & f(\mathbf{Y}^n + a_{41}\boldsymbol{\Delta}_1 + a_{42}\boldsymbol{\Delta}_2 + a_{43}\boldsymbol{\Delta}_3) \\ & + (c_{41}\boldsymbol{\Delta}_1 + c_{42}\boldsymbol{\Delta}_2 + c_{43}\boldsymbol{\Delta}_3)/h. \end{aligned} \tag{11}$$

Cooling

- Cooling by molecular hydrogen ($T < 10^4$ K)

$H_2 + D^+ \rightarrow HD + H^+$ exothermic,

and

$HD + H^+ \rightarrow H_2 + D^+.$ endothermic

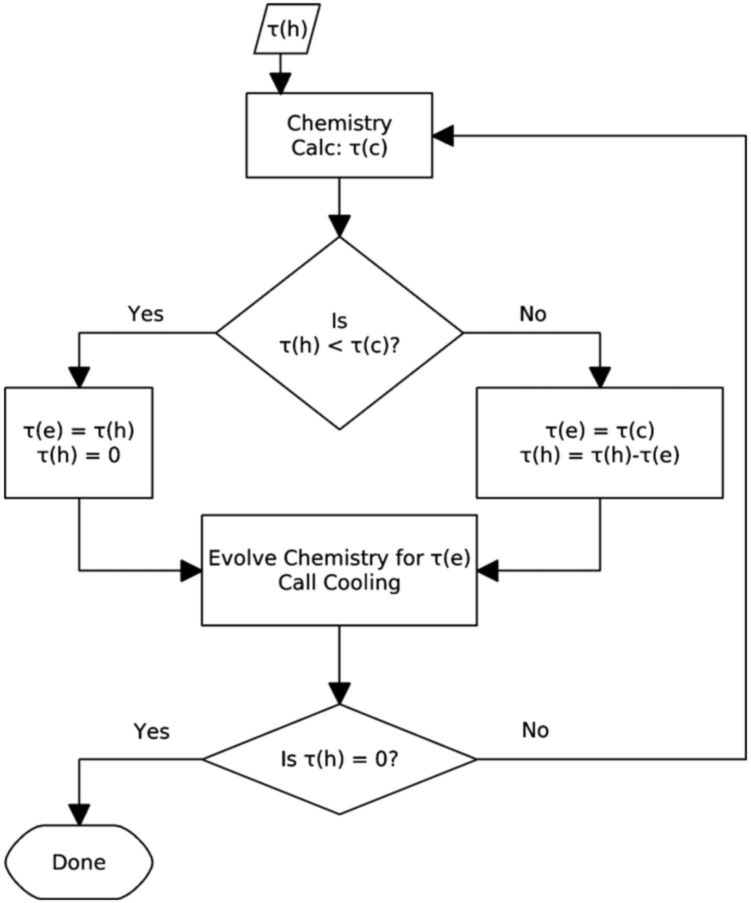
- Cooling by atomic line emission ($T > 10^4$ K)

Time Step Control

$$\tau_{\mathrm{chem},i} = \alpha_{\mathrm{chem}} \frac{Y_i + 0.1 Y_{H^+}}{\dot{Y}_i}, \tag{12}$$

$$\tau_{\mathrm{cool}} = \frac{\alpha_{\mathrm{cool}} \times E_i}{\dot{s}}, \tag{15}$$

Time Step Control


τ(h)

Chemistry
Calc: τ(c)

Is
τ(h) < τ(c)?

Yes

τ(e) = τ(h)
τ(h) = 0

No

τ(e) = τ(c)
τ(h) = τ(h)-τ(e)

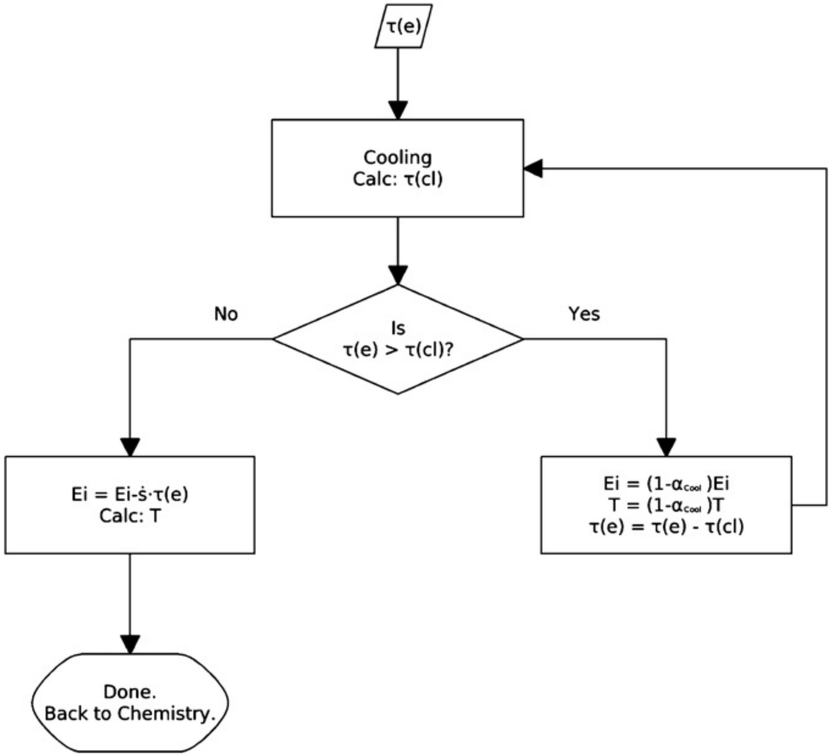
Evolve Chemistry for τ(e)
Call Cooling

Is τ(h) = 0?

Yes

Done

No


τ(e)

Cooling
Calc: τ(cl)

Is
τ(e) > τ(cl)?

No

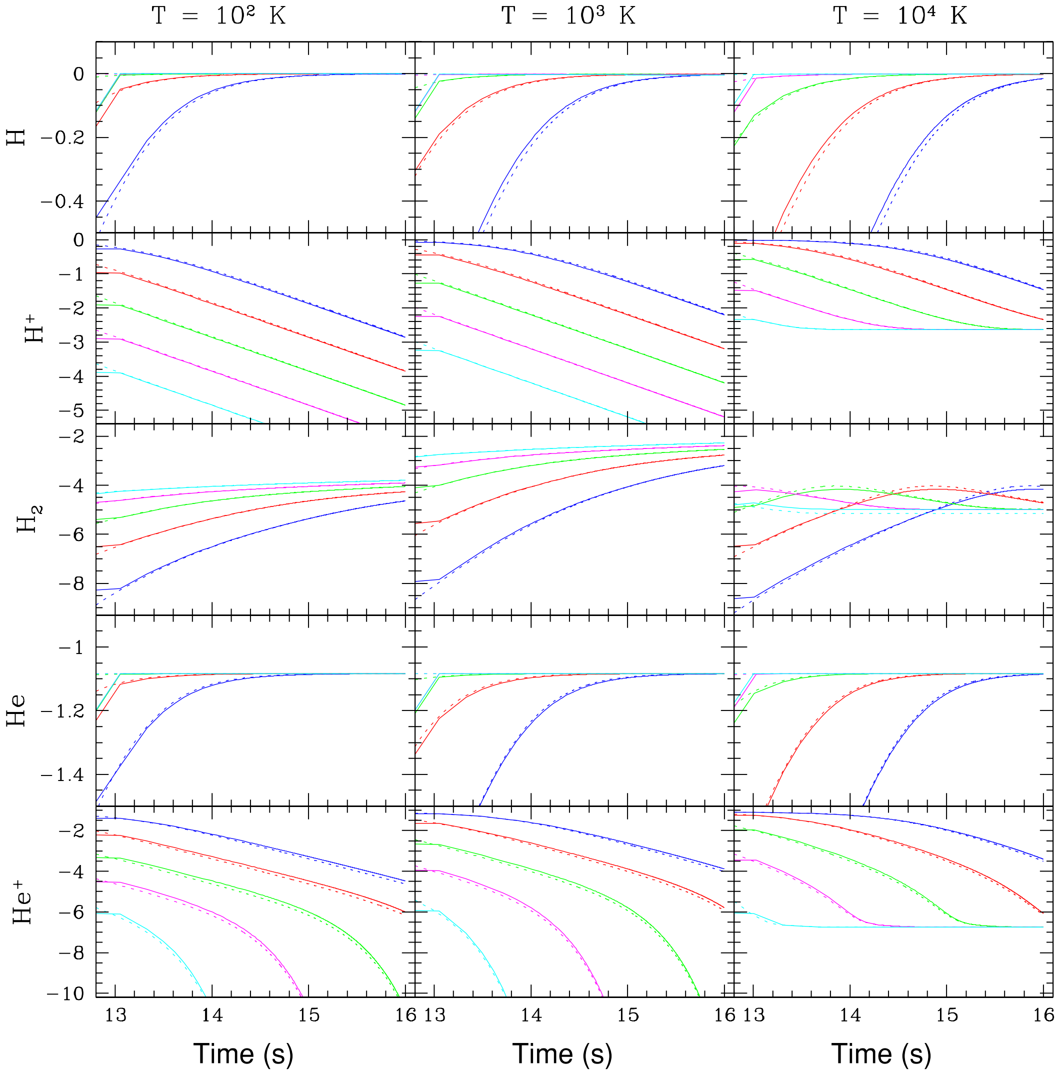
Ei = Ei-$\dot{s}$·τ(e)
Calc: T

Done.
Back to Chemistry.

Yes

Ei = (1-α_{cool})Ei
T = (1-α_{cool})T
τ(e) = τ(e) - τ(cl)

Code Test: Chemical Evolution



Code Test: Cooling

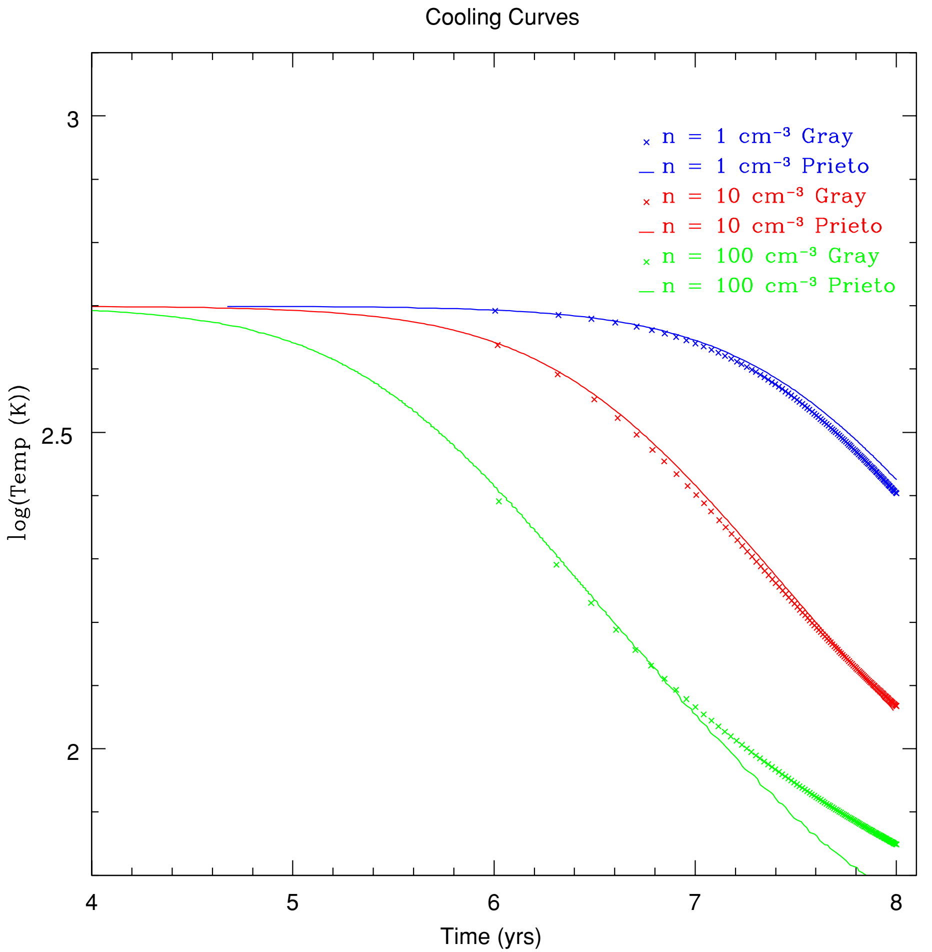


Figure 5. Cooling tests. The solid lines are taken from Prieto et al. (2009) and compared to our model. The blue curves correspond to a number density $n = 1.0\ \mathrm{cm}^{-3}$, red to $n = 10.0\ \mathrm{cm}^{-3}$, and green to $n = 100.0\ \mathrm{cm}^{-3}$. The temperature is not allowed to go below 50 K.

Model Simulations

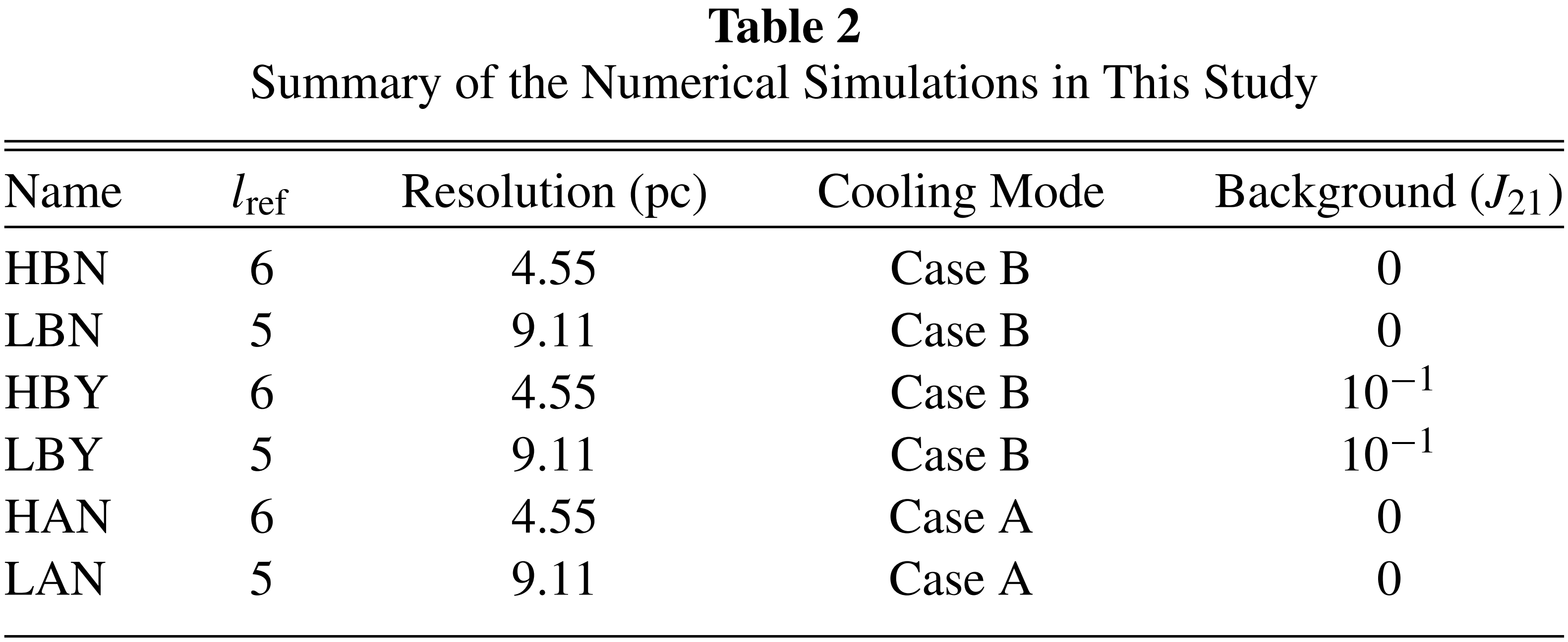
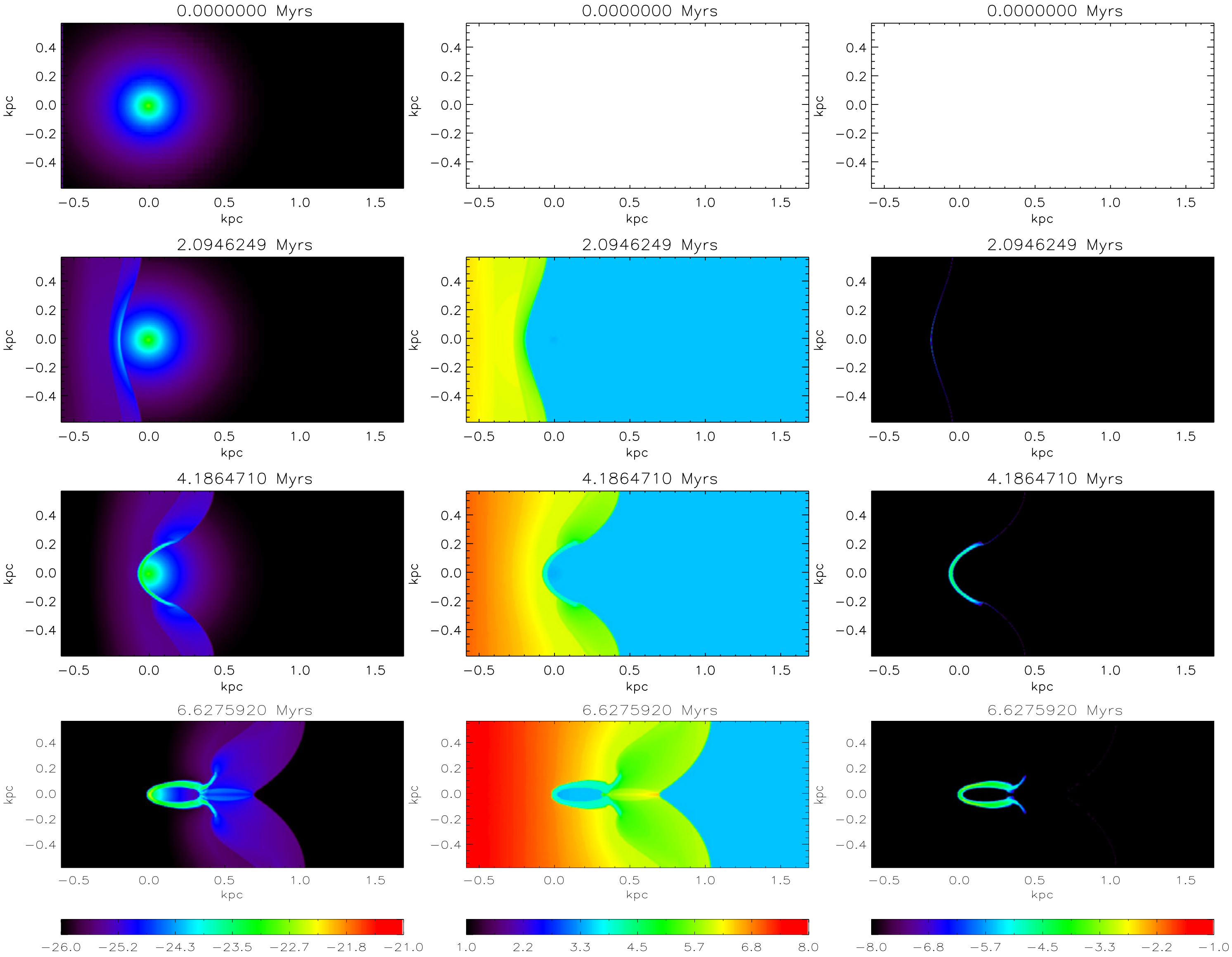


Table 2

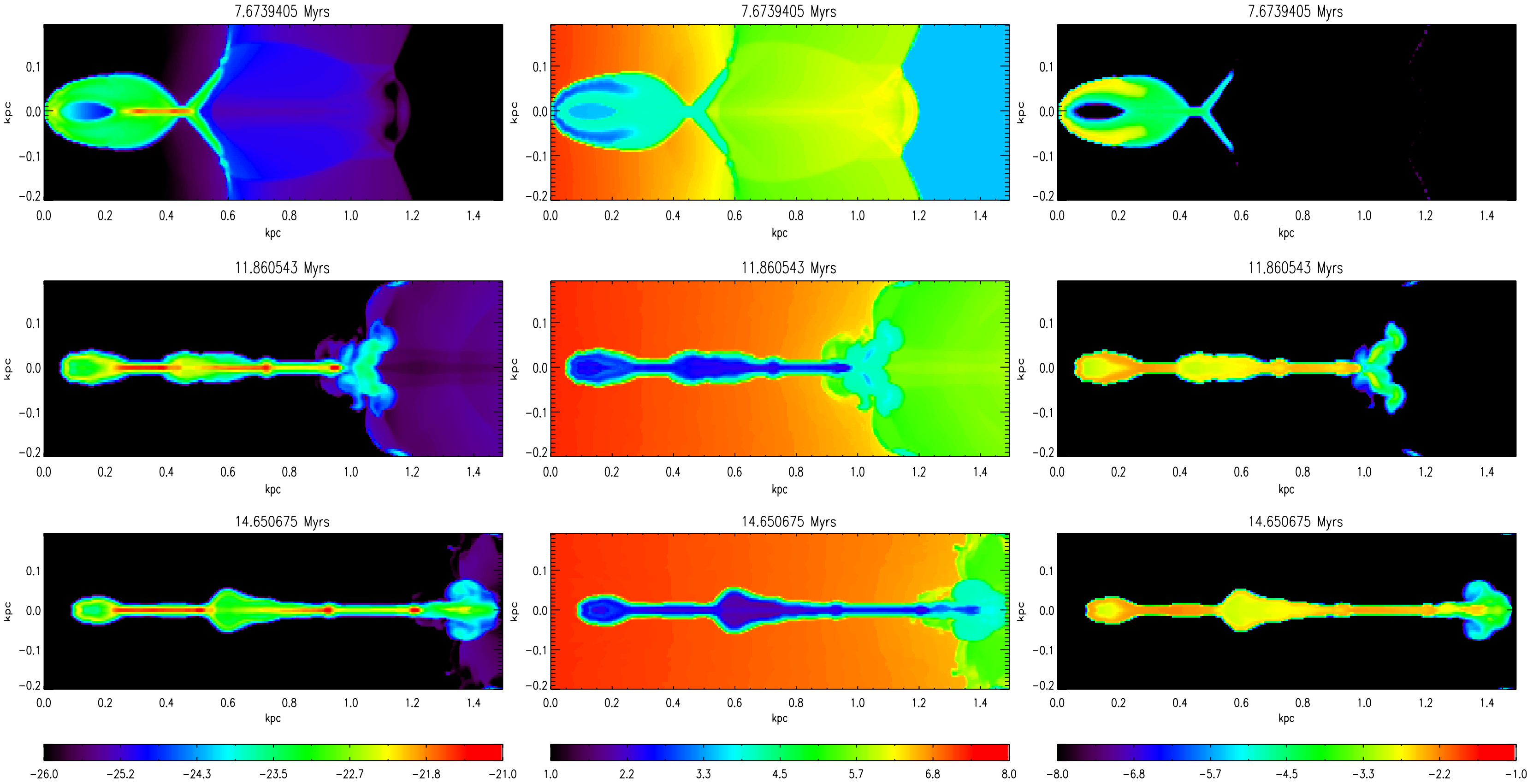
Summary of the Numerical Simulations in This Study

Name	l_{ref}	Resolution (pc)	Cooling Mode	Background (J_{21})
HBN	6	4.55	Case B	0
LBN	5	9.11	Case B	0
HBY	6	4.55	Case B	10^{-1}
LBY	5	9.11	Case B	10^{-1}
HAN	6	4.55	Case A	0
LAN	5	9.11	Case A	0

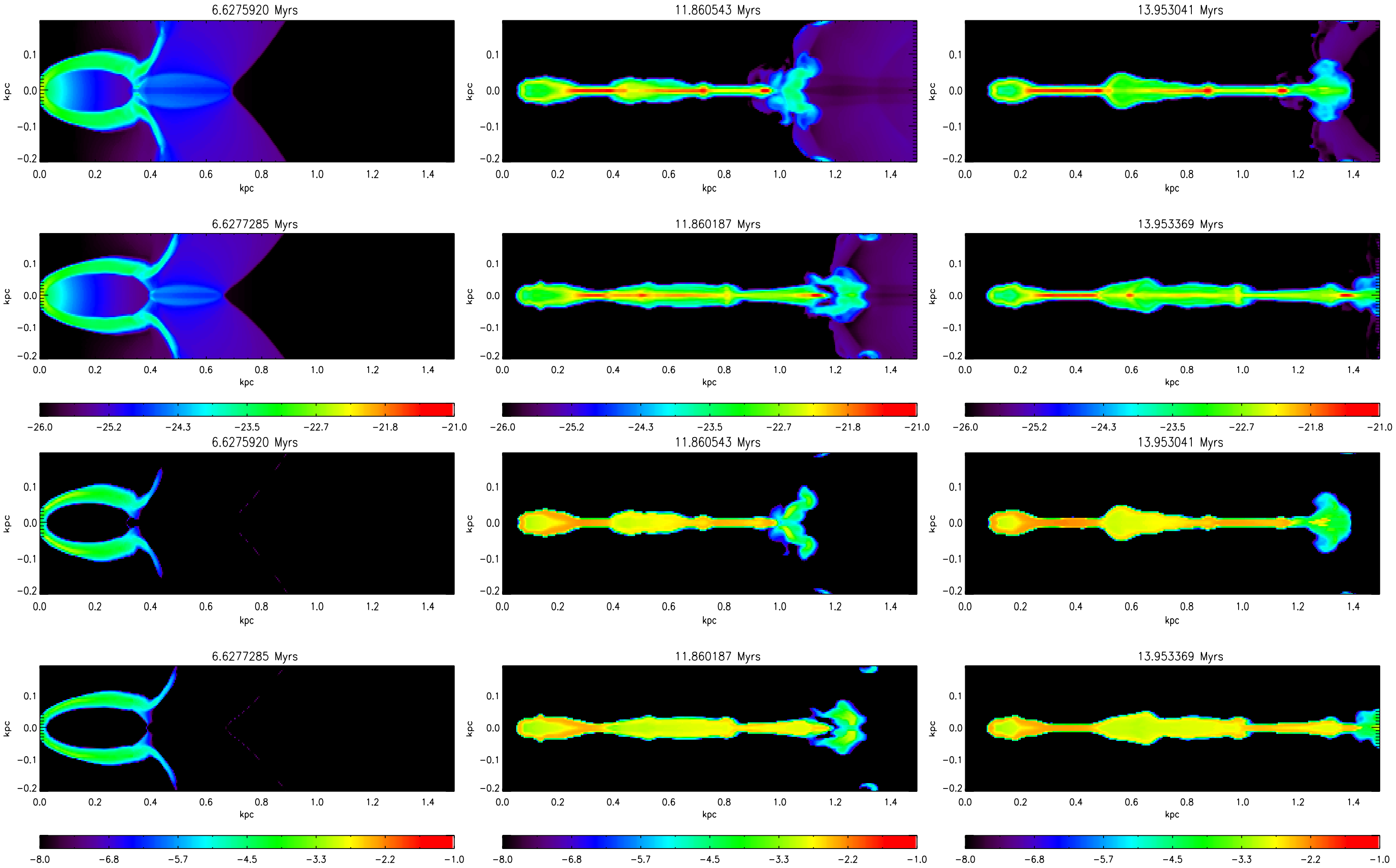
Results: Reference Run



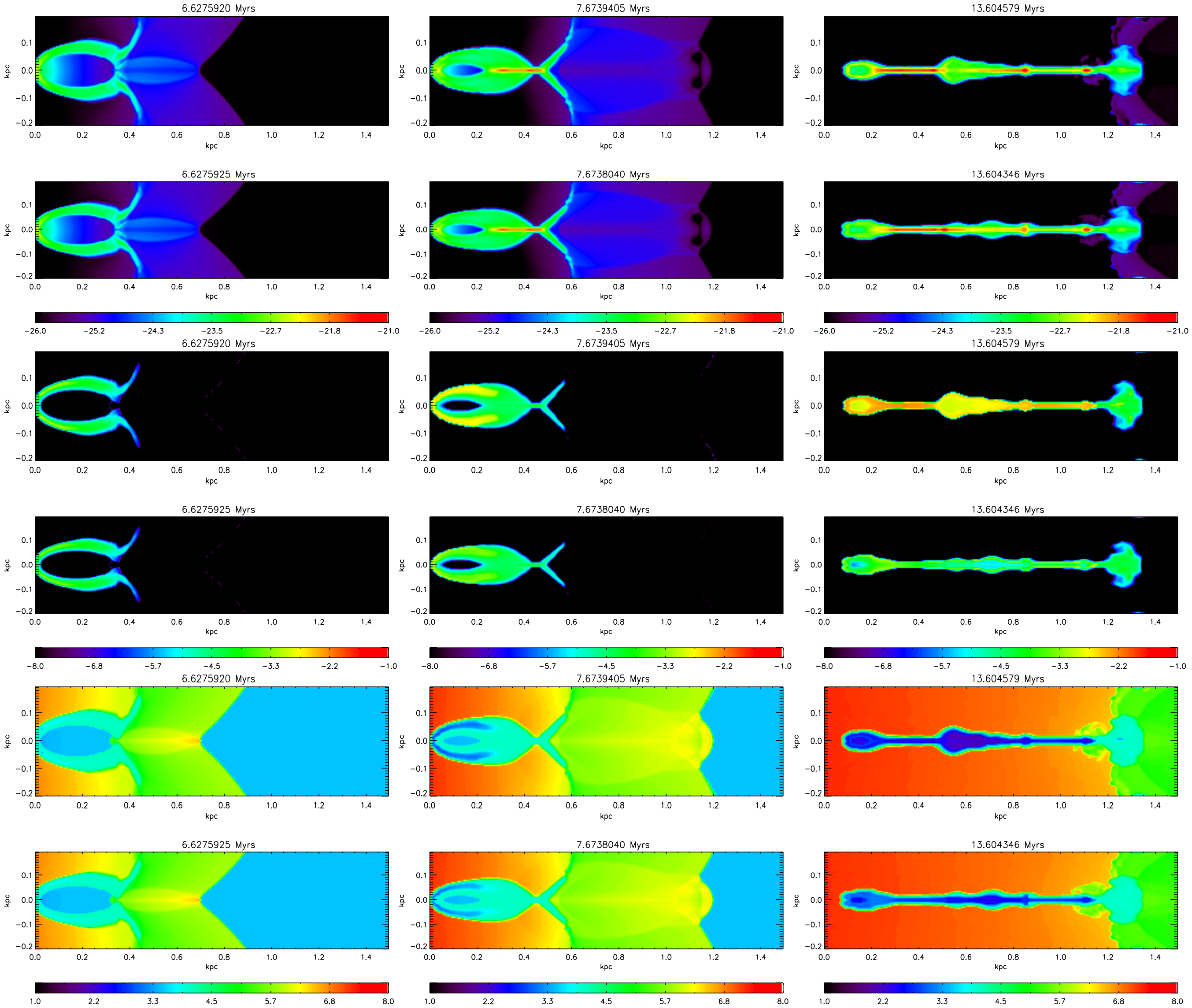
Results: Reference Run



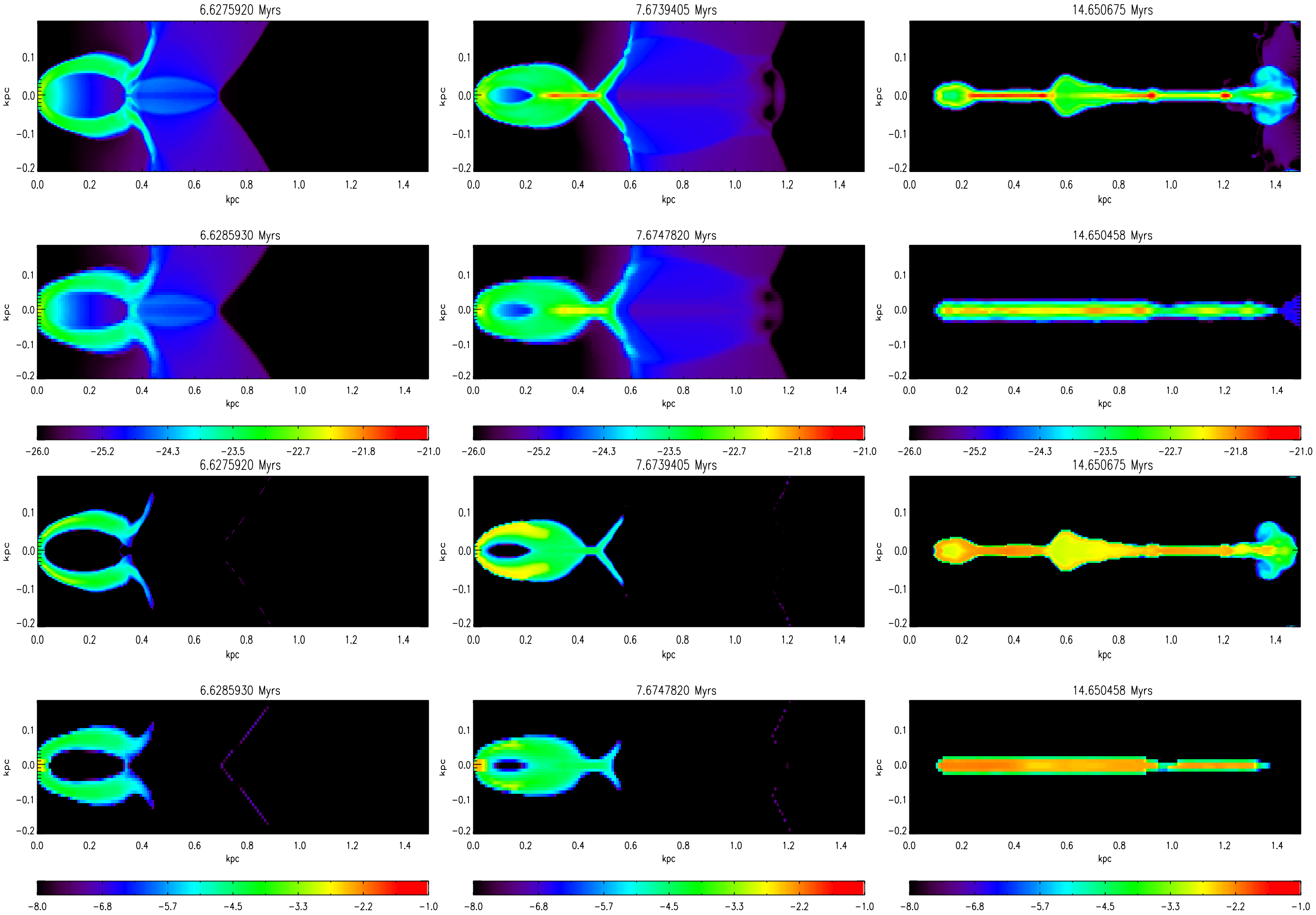
Results: Effect of Optical Depth



Effect of Background Radiation



Effect of Simulation Resolution



Formation of Stellar Cluster