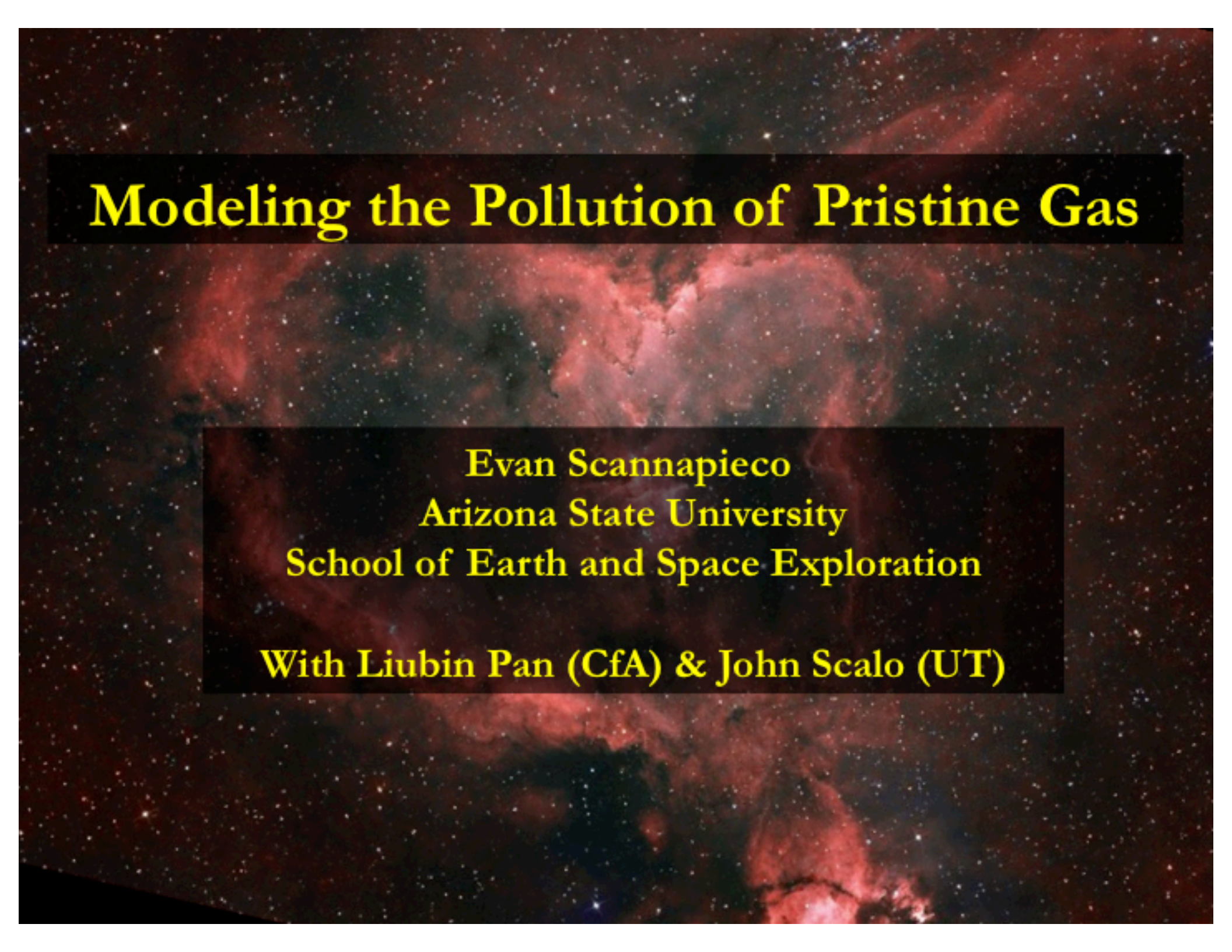


# **Modeling the Pollution of Pristine Gas**

**Evan Scannapieco**  
**Arizona State University**  
**School of Earth and Space Exploration**  
**With Liubin Pan (CfA) & John Scalo (UT)**

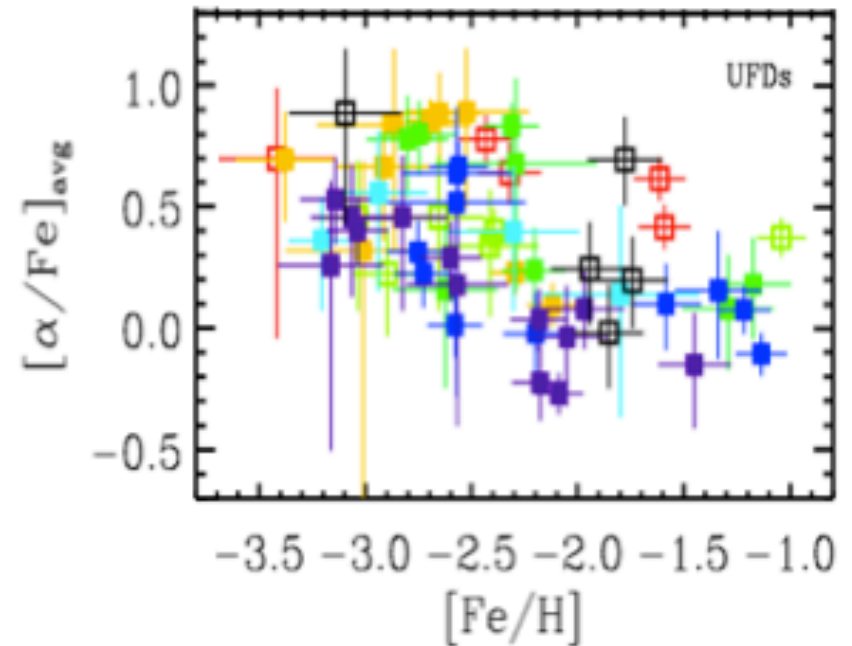
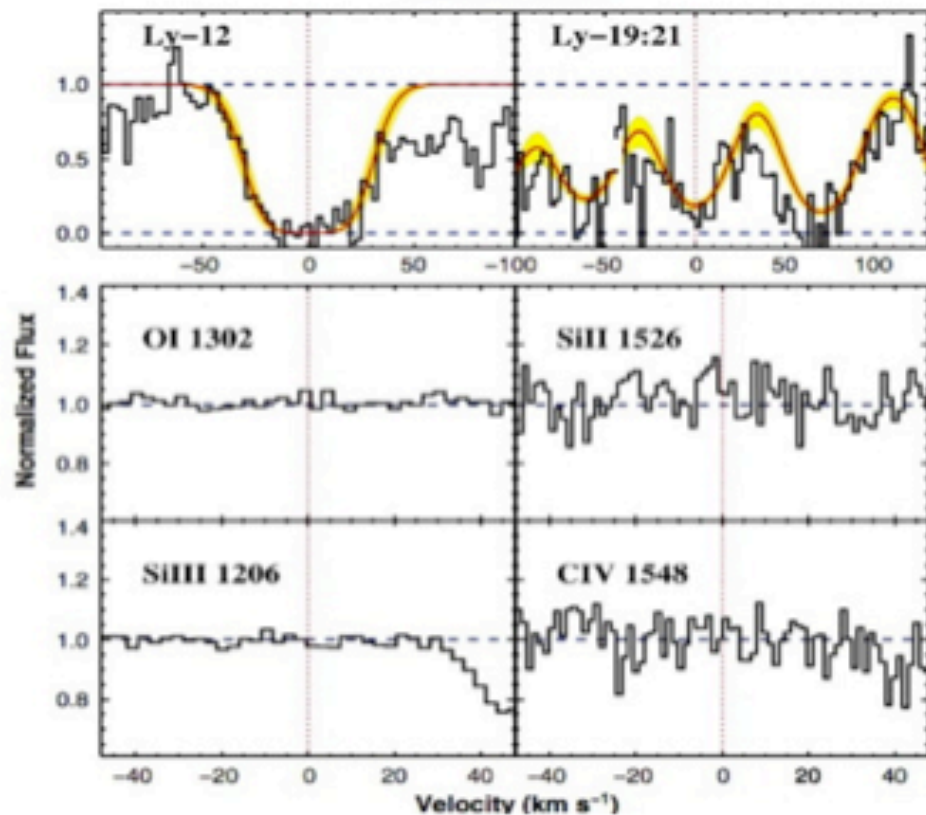


# **Modeling the Pollution of Pristine Gas**

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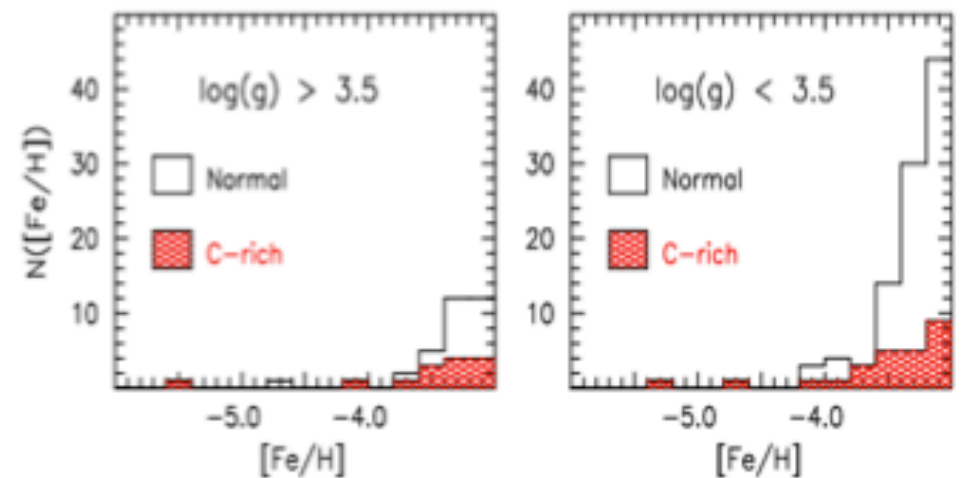
**With Liubin Pan (CfA) & John Scalo (UT)**

# Evolution of the Metal-Free Fraction



Vargas, Geha, Kirby, & Simon (2013)

	LLS1134a	LLS05968
Redshift	$3.410883 \pm 0.000004$	$3.096221 \pm 0.000009$
$\log N_{\text{H}}$	$17.95 \pm 0.05$	$17.18 \pm 0.04$
$\log D/\text{H}$	$-4.69 \pm 0.13^*$	-
$b_{\text{H I}}$ (km s <sup>-1</sup> )	$15.4 \pm 0.3$	$20.2 \pm 0.8$
Temperature (K)	$< (1.43 \pm 0.05) \times 10^4$	$< (2.48 \pm 0.19) \times 10^4$
Metallicity ( $Z_{\odot}$ )	$< 10^{-4.2}$	$< 10^{-3.8}$
$\log x_{\text{He}}$	$\leq 2.10$	$\leq 2.40$
$\log n_{\text{H}}$	$\leq 1.86$	$\leq 1.98$
$\log U^{\dagger}$	$\geq 3$	$\geq 3$

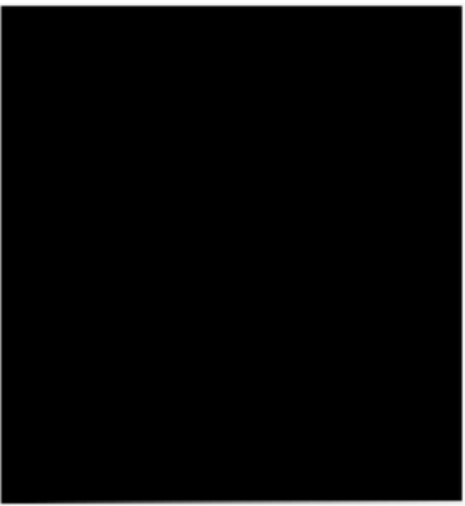
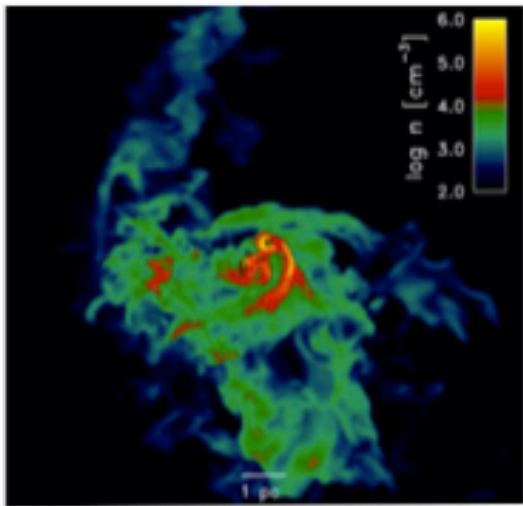
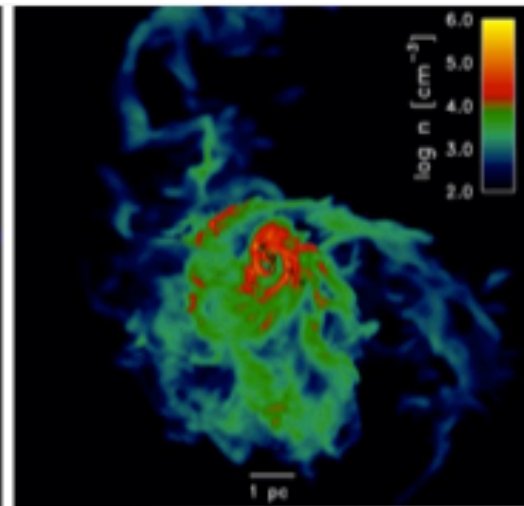


Frebel & Norris (2013)

Fumagalli et al (2011) see also Simcoe (2012)

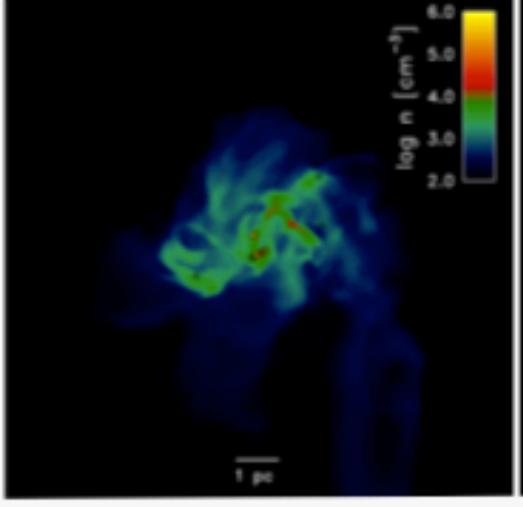
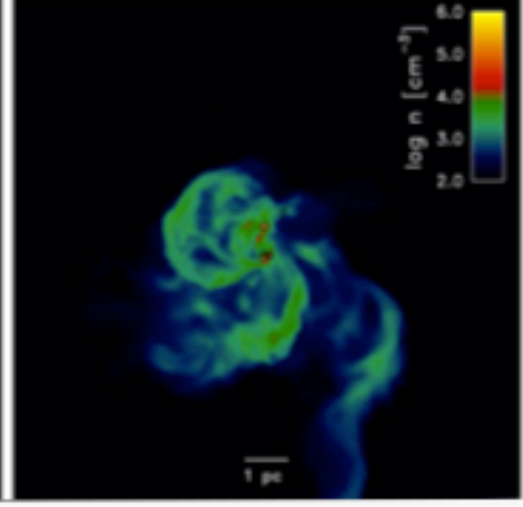
$10^{-2} Z_{\odot}$

$\log n \text{ [cm}^{-3}\text{]}$



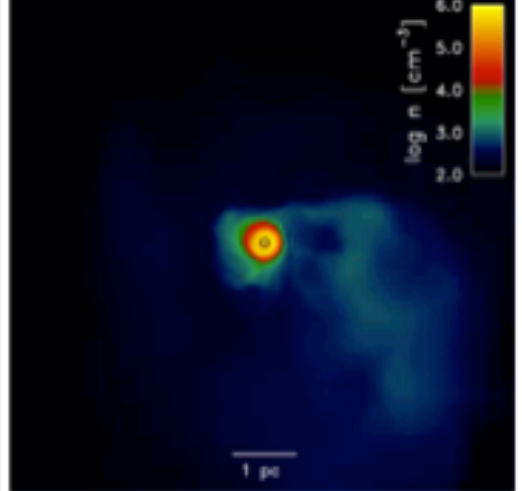
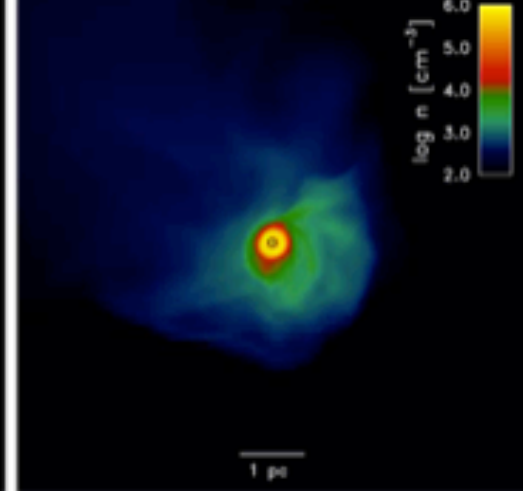
$10^{-3} Z_{\odot}$

$\log n \text{ [cm}^{-3}\text{]}$



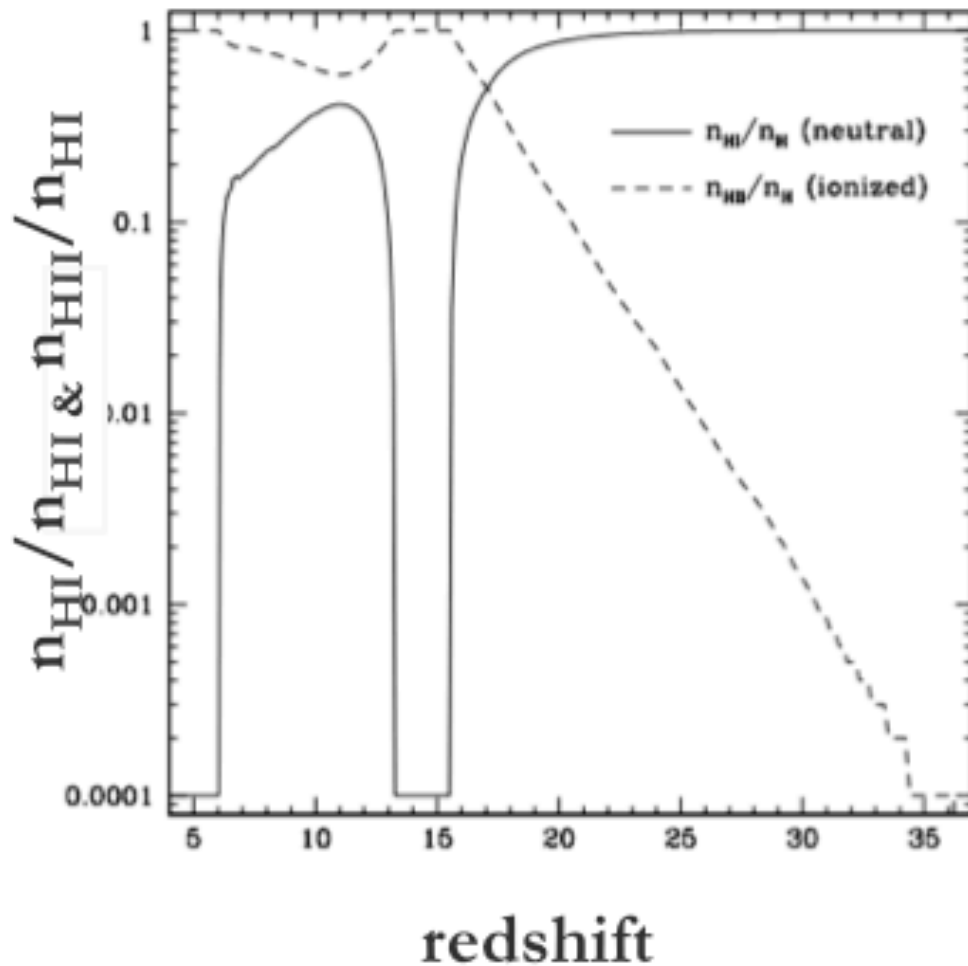
$10^{-4} Z_{\odot}$

$\log n \text{ [cm}^{-3}\text{]}$

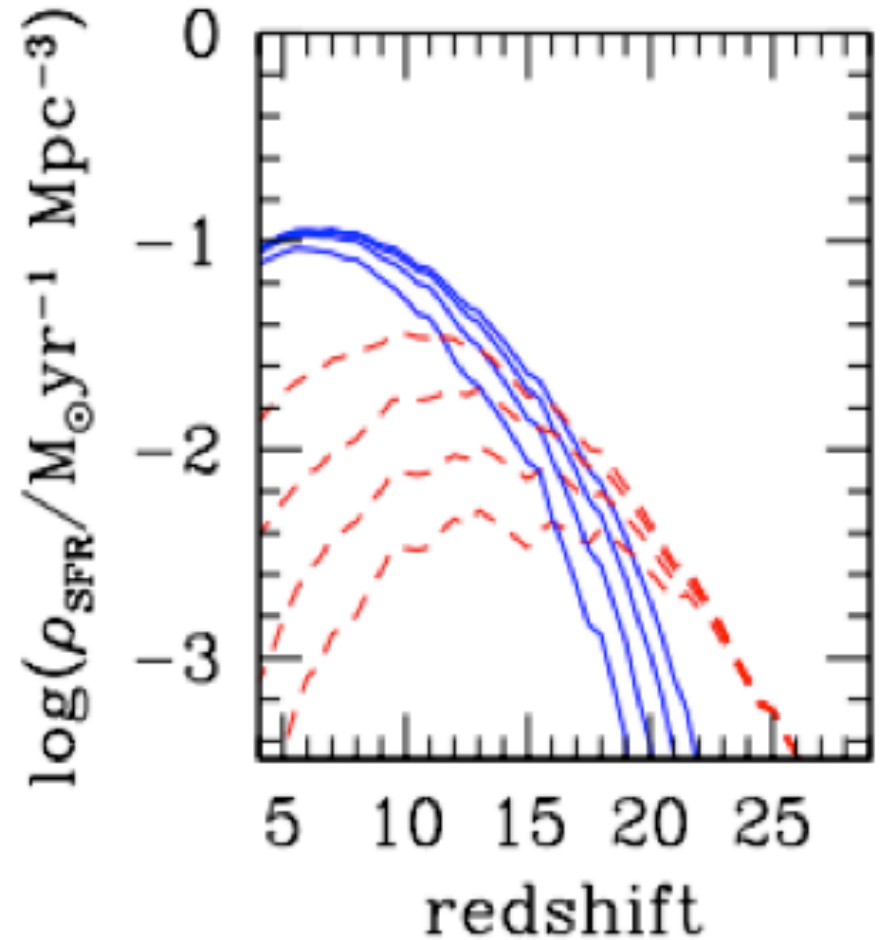


Safronek-Shrader,  
Milosavljevic,  
& Bromm (2014)

# Population III -> II Transition

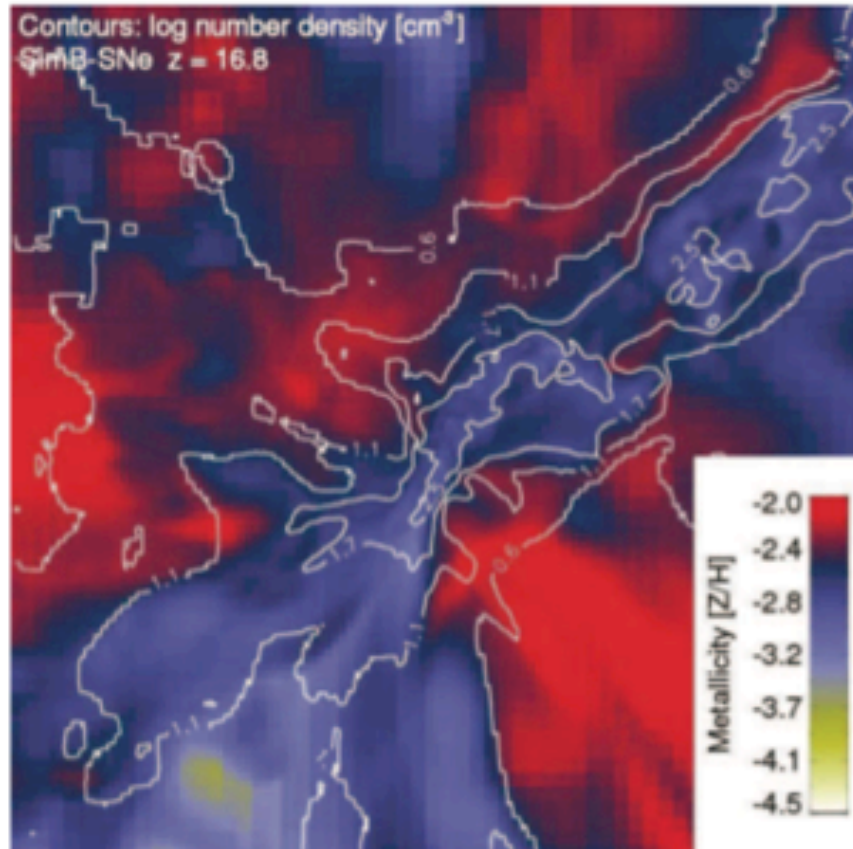


Cen (2003)



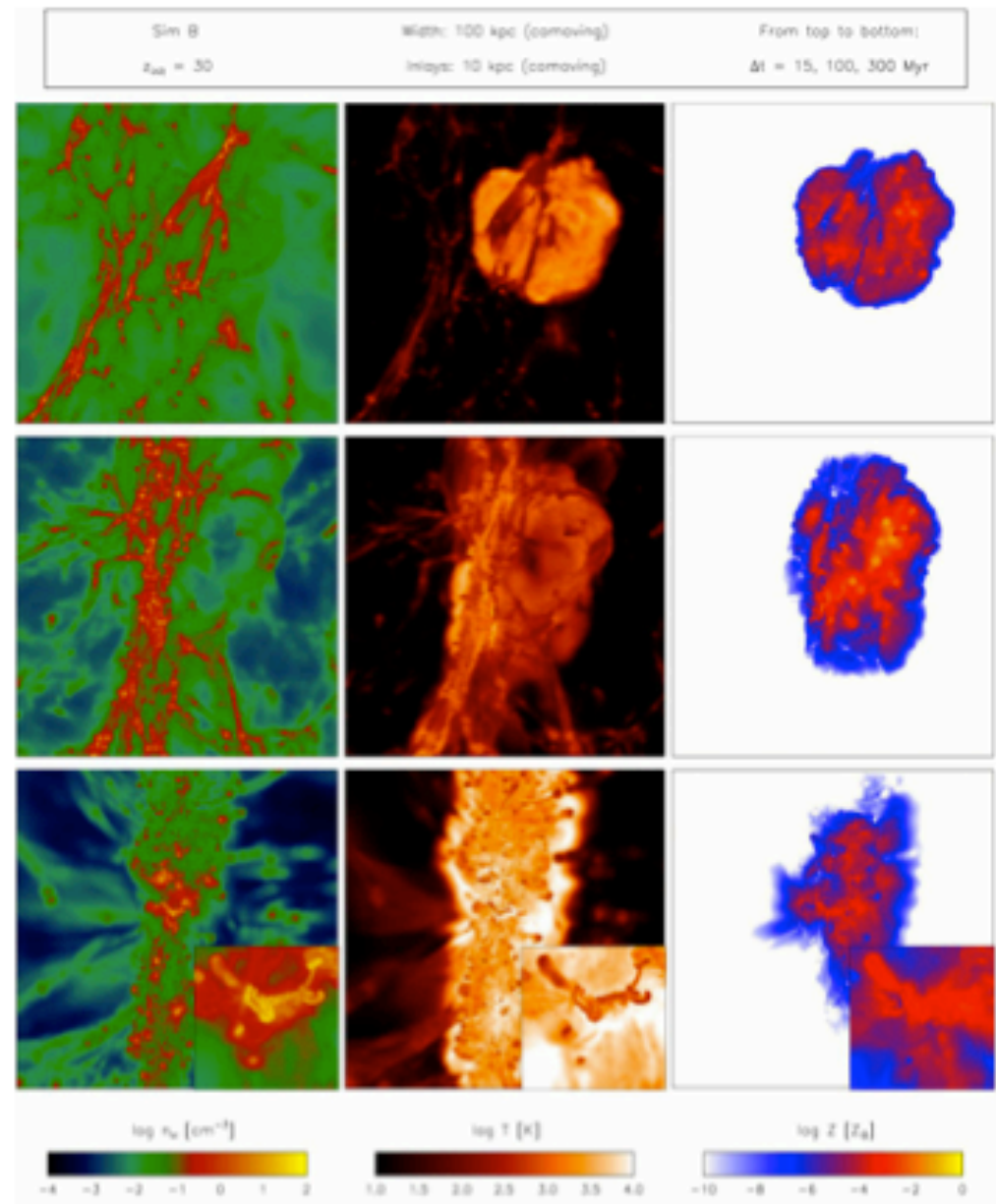
ES, Schneider, & Ferrara (2003)

# Population III -> II Transition



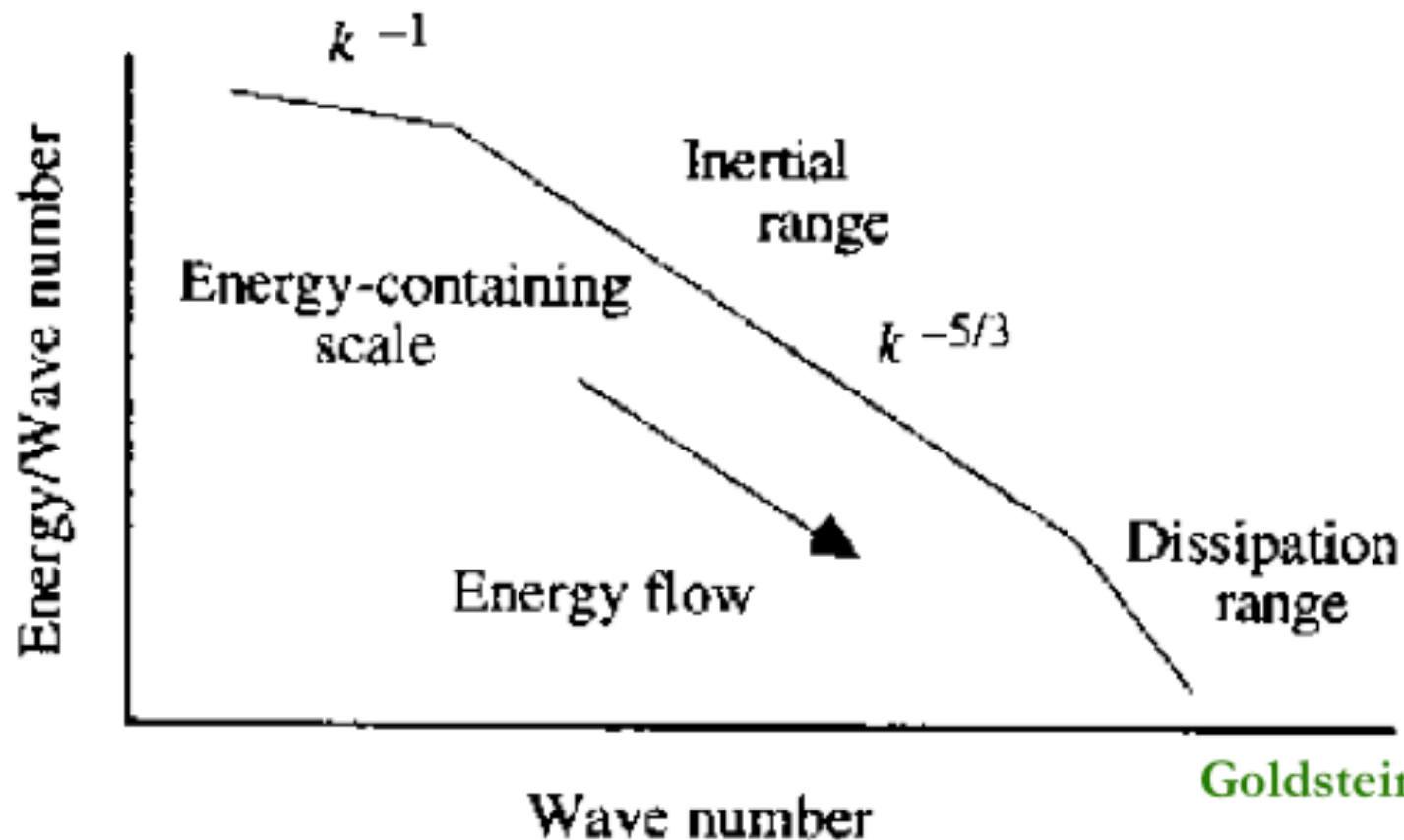
Wise & Abel (2008)

See also Ritter, Safranek-Shrader,  
Gnat, Milosavlkevic, & Bromm (2012)



Greif, Glover, Bromm, & Klessen (2010)

# Mixing is Driven by (Unresolved) Turbulence



**Ionized Medium**

Spitzer :

$$L \approx 10^{-2} \text{ pc } V_{10} n^{-1} T_5^{5/2}$$

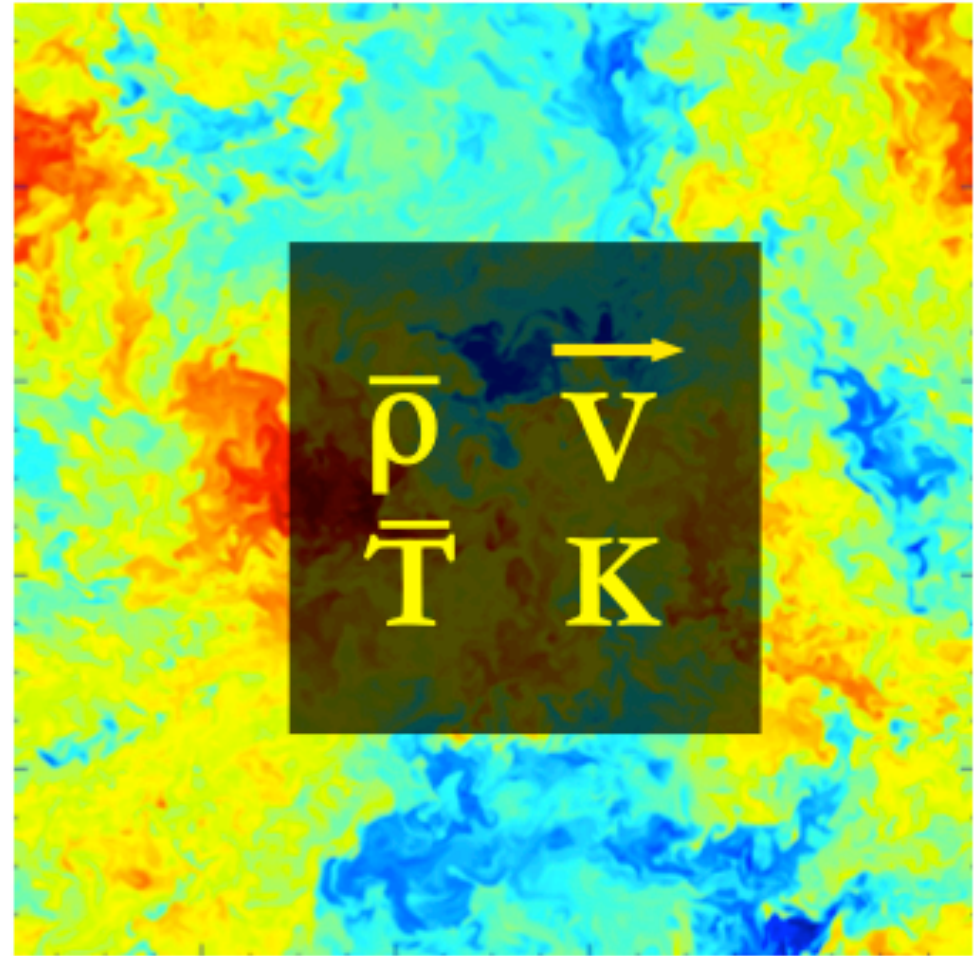
**Neutral Medium**

Ambipolar Diffusion :

$$L \approx 10^{-3} \text{ pc } V_{A,10} n^{-1} / \alpha_{-6}$$

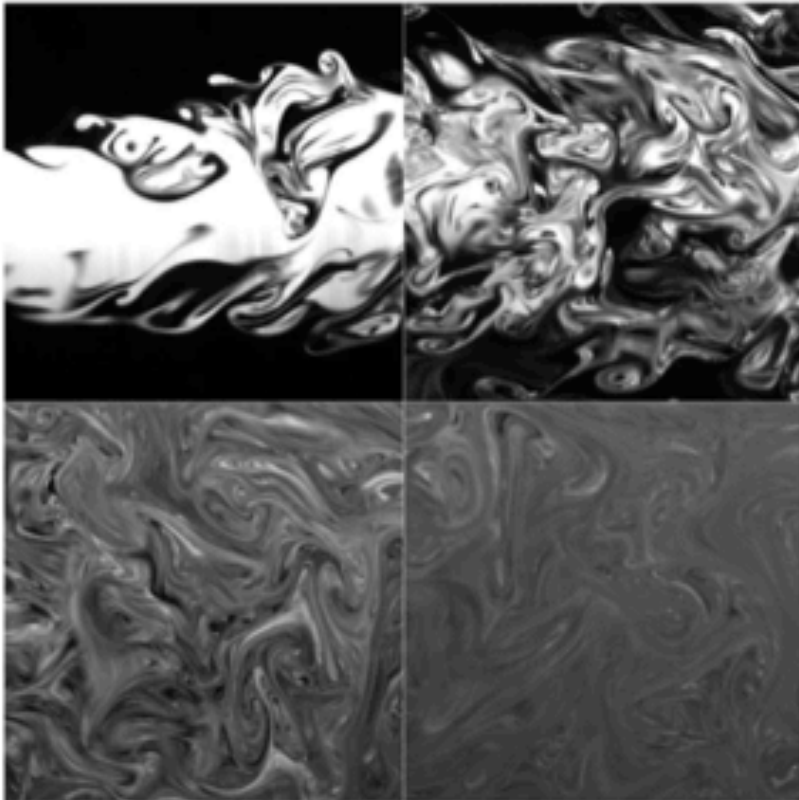
# Mixing is Driven by (Unresolved) Turbulence

$\vec{v}$   
 $\rho$   
 $T$   
 $P(\rho, T)$





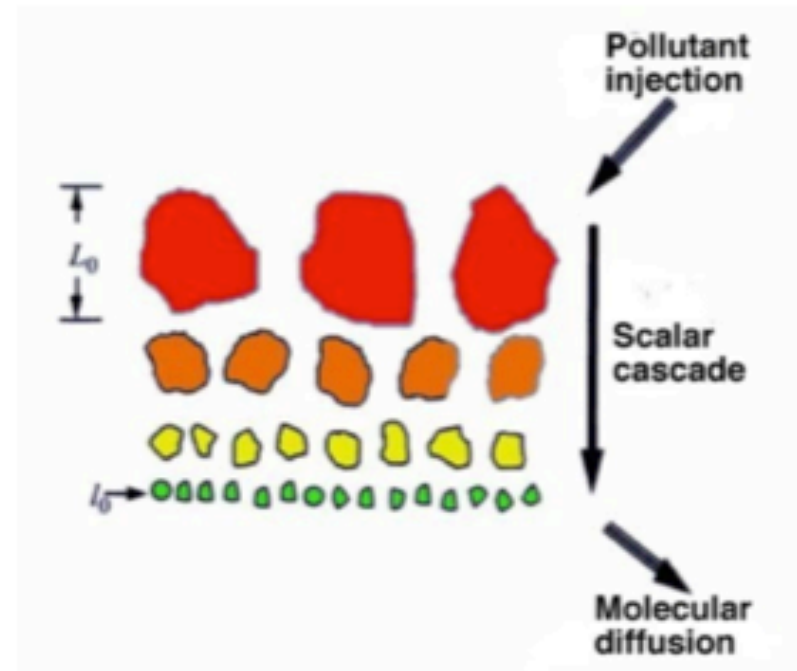
# Turbulent Mixing



Mixing of a jet of dye

Duplat & Villermaux (2008)

Classic phenomenology (Obukohov-Corrsin)



$$\text{Mixing timescale } \tau_{\text{mix}} \sim L/V_t$$

# Simulations

The FLASH code with modified “Stir unit” for flow and scalar driving

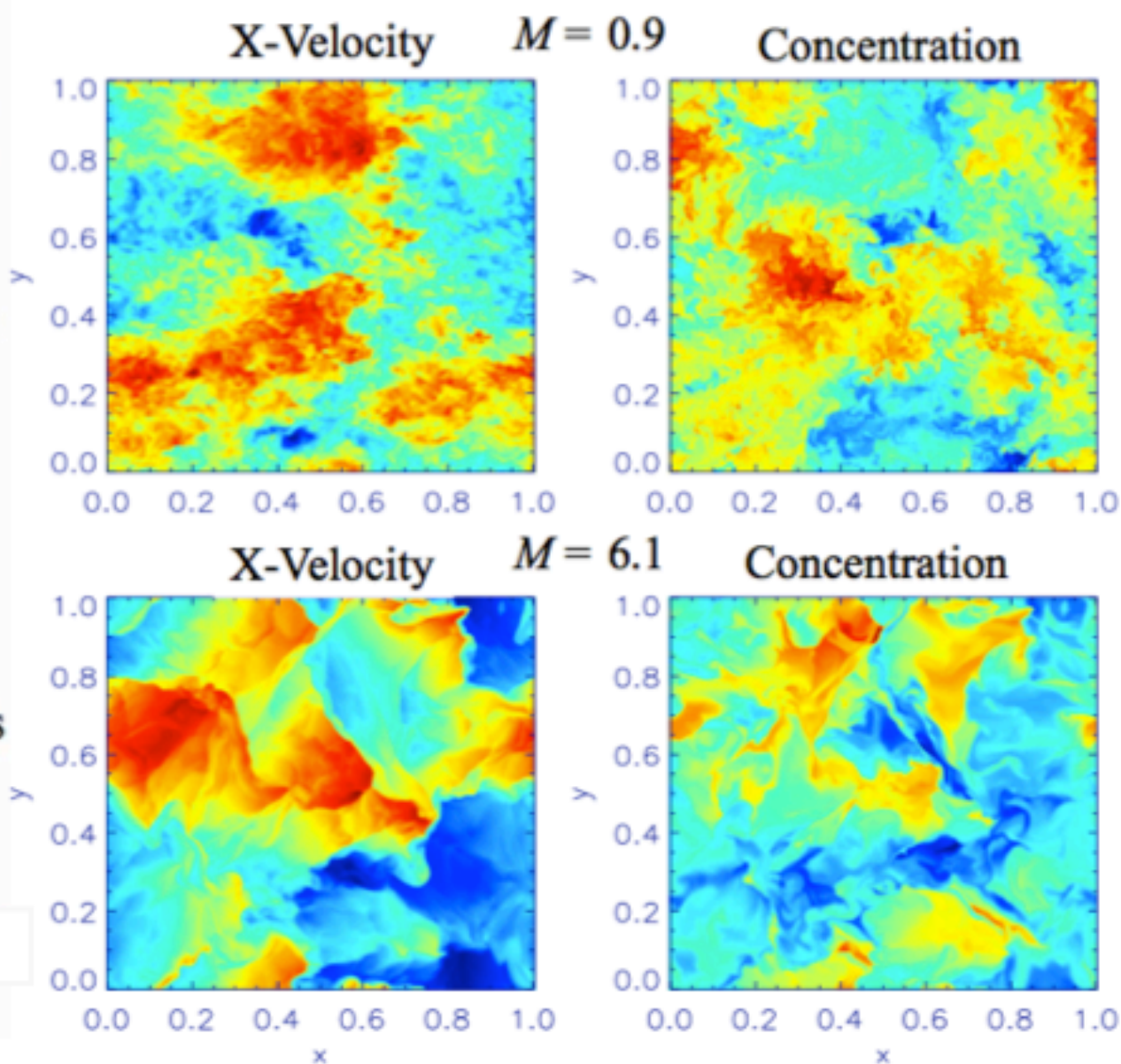
A periodic box of unit size with  $512^3$  cells.

Solenoidal external force with  $2\pi \leq k \leq 6\pi$

Isothermal equation of state

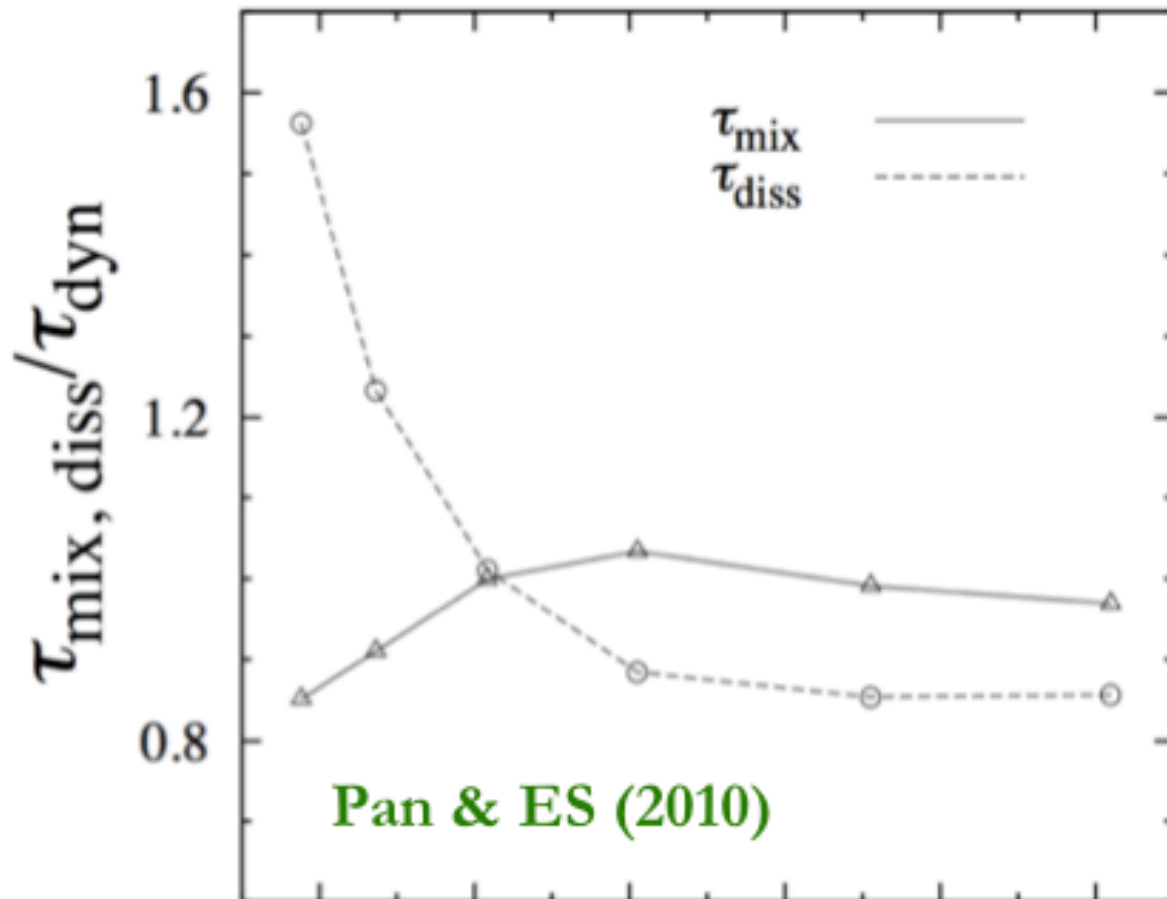
Six flows with Mach numbers  $0.9 \leq M \leq 6.1$

The same forcing pattern for scalar sources



Pan & ES (2010)

# Mixing Timescales



- Energy dissipation rate increases with Mach #
- Mixing rate decreases with M: compressible modes are less efficient at producing small scalar structures.

$$\partial_t \langle \tilde{\rho} C^2 \rangle + \partial_i \langle \tilde{\rho} C^2 v_i \rangle = 2 \langle \partial_i (\tilde{\rho} \kappa C \partial_i C) \rangle + 2 \langle \tilde{\rho} S C \rangle$$

↑  
Advection term

↑  
Diffusivity term

↑  
Source term

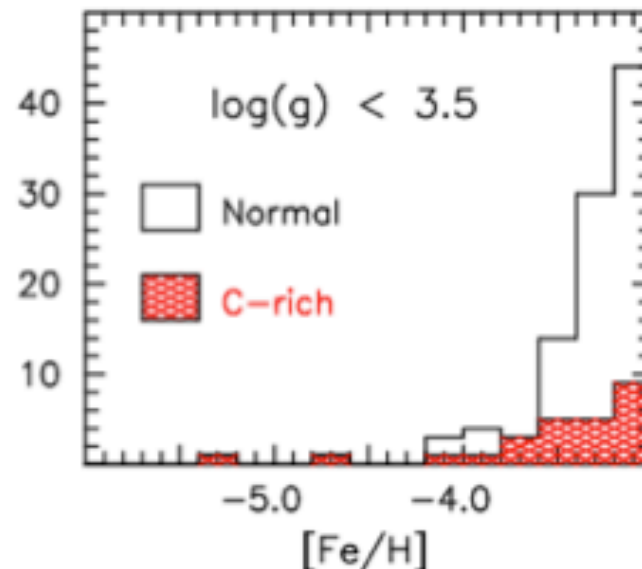
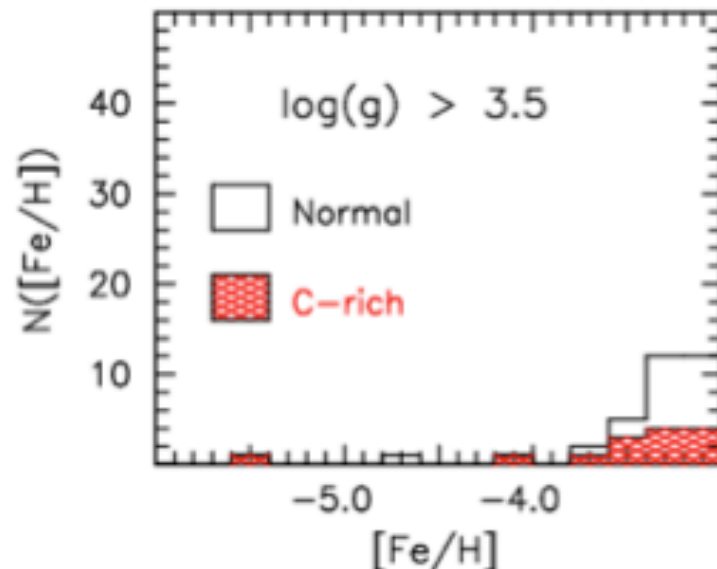
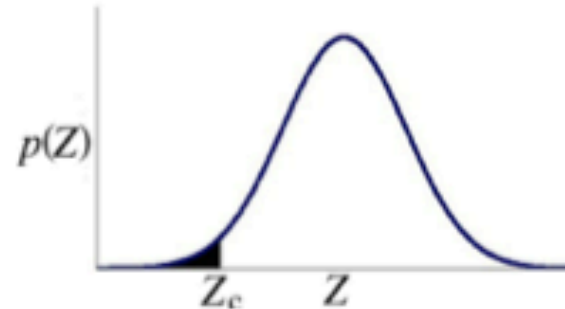
## But what about the extremes?

- Define a density-weighted concentration PDF,

$$p(Z; t)$$

then the mass fraction of the flow with  $Z < Z_c$  ( $\sim 10^{-8} - 10^{-5}$ ) is,

$$P(Z_c, t) = \int_0^{Z_c} p(Z'; t) dZ'$$



Frebel & Norris (2013)

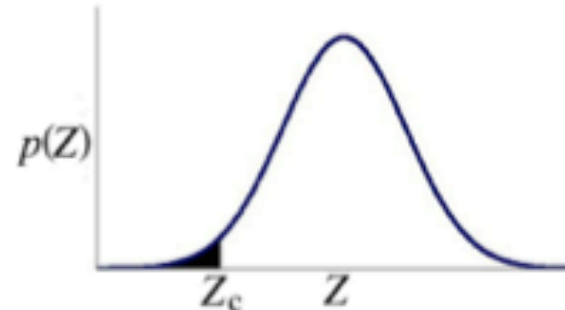
## But what about the extremes?

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$$P(Z_c, t) = \int_0^{Z_c} p(Z'; t) dZ'$$



- From the concentration equation and the continuity equation, one can derive the PDF equation,

$$\frac{\partial p(Z; \mathbf{x}, t)}{\partial t} + \nabla \cdot \left( p \frac{\langle \rho \mathbf{v} | C = Z \rangle}{\langle \rho | C = Z \rangle} \right) = - \frac{\partial}{\partial Z} \left( p \frac{\langle \nabla \cdot (\rho \kappa \nabla C) | C = Z \rangle}{\langle \rho | C = Z \rangle} \right) - \frac{\partial}{\partial Z} \left( p \frac{\langle \rho S | C = Z \rangle}{\langle \rho | C = Z \rangle} \right)$$

↑  
Advection term

↑  
Diffusivity term

↑  
Source term

# Closure Models

Nonlinear integral models (Curl 1963; Dopazo 1979; Janicka et al. 1979)



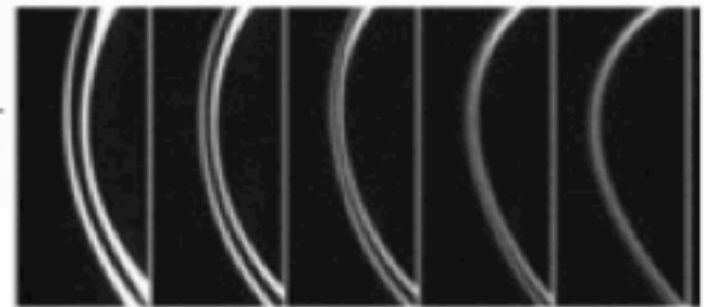
# Closure Models

Nonlinear integral models (Curl 1963; Dopazo 1979; Janicka et al. 1979)

$$\frac{\partial p(Z;t)}{\partial t} = \gamma(t) \left\{ \left[ \int_0^1 dZ_1 p(Z_1;t) \int_0^1 dZ_2 p(Z_2;t) \delta \left( Z - \frac{Z_1 + Z_2}{2} \right) \right] - p(Z;t) \right\}$$

Stretching  $\rightarrow$  Scalar sheets  $\rightarrow$  Mixing

$$\frac{dP(t)}{dt} = -\frac{P(1-P)}{\tau_{\text{int}}} \rightarrow P(t) = \frac{P_0}{P_0 + (1-P_0) \exp\left(\frac{t}{\tau_{\text{int}}}\right)}$$



Self-convolution models (Venaille & Sommeria 2007; Villermaux & Duplat 2008)

$\rightarrow$  Continuous convolution model:

$$\frac{dP(t)}{dt} = \frac{P \ln(P)}{\tau_{\text{con}}}$$

$$\rightarrow P(t) = P_0^{\exp(t/\tau_{\text{con}})}$$

$\rightarrow$  Generalized convolution model:

$$\frac{dP}{dt} = -\frac{n}{\tau_{\text{con}}} P(1 - P^{1/n})$$

$$\rightarrow P(t) = \frac{P_0}{\left[ P_0^{1/n} + (1 - P_0^{1/n}) \exp(t/\tau_{\text{con}}) \right]^n}$$

# Initial Conditions

Set to be bimodal (purely polluted, and purely pristine):

$$p(Z;0) = P_0 \delta(Z) + H_0 \delta(Z-1),$$

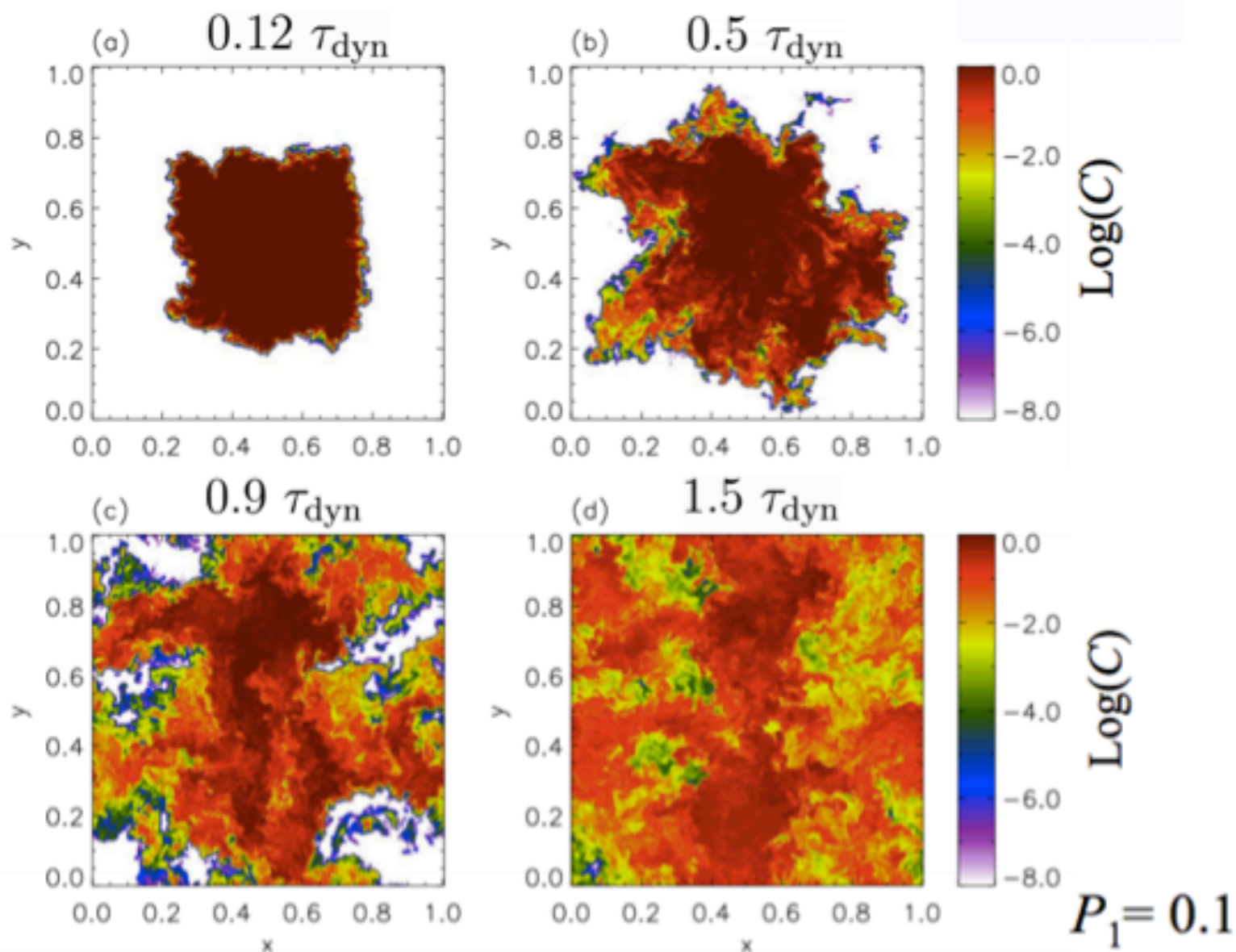
where  $P_0$  and  $H_0$  are the initial pristine and pollutant fractions.

Initial Pollutant region is a cube at the center of the box

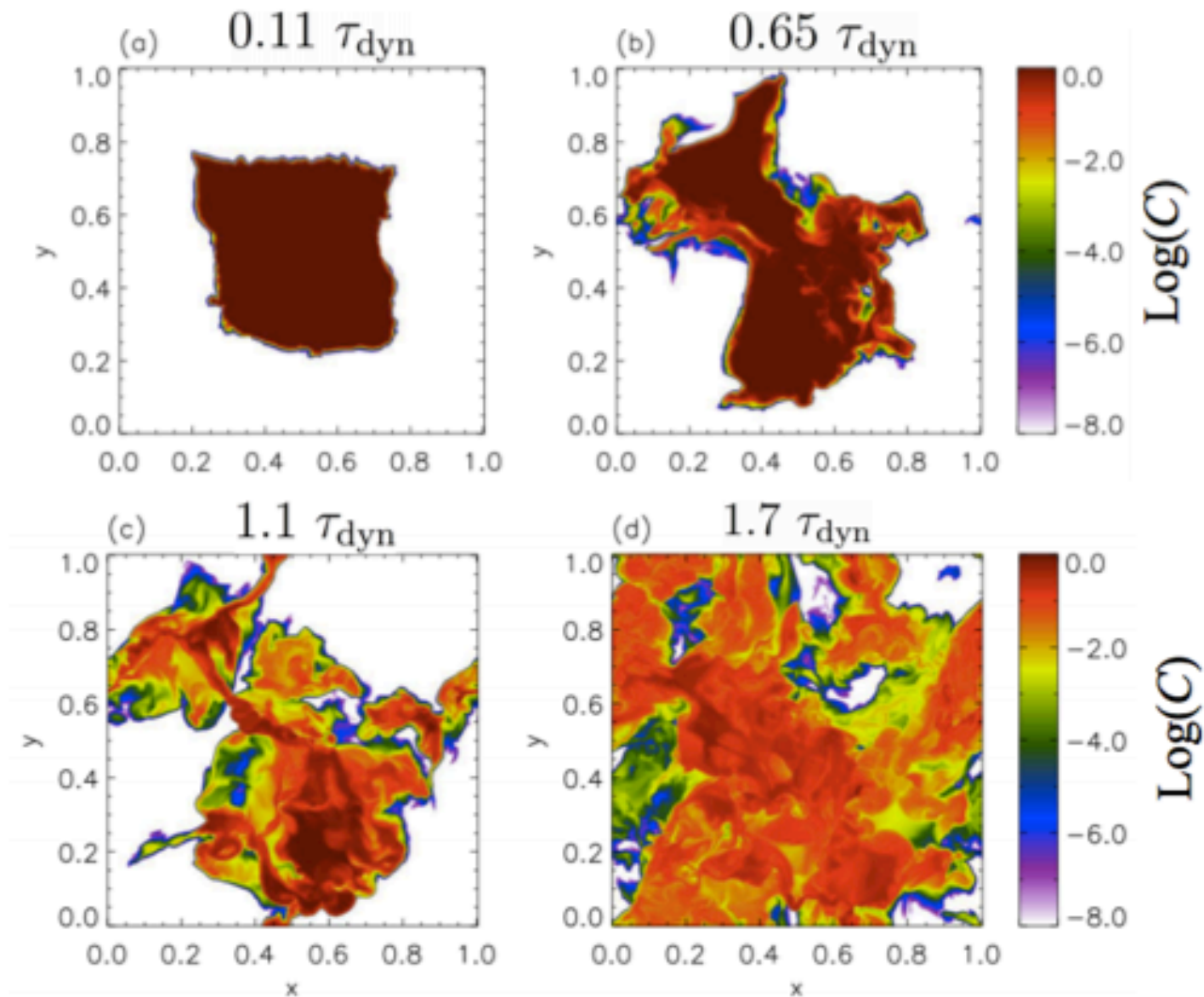
Category	Pollutant Configuration	$H_0 = 0.5$	$H_0 = 0.1$	$H_0 = 10^{-2}$	$H_0 = 10^{-3}$
i	1 cube	iA	iB	iC	iD
ii	1 ball	iiA	iiB	iiC	iiD
iii	$2^3$ balls	iiiA	iiiB	iiiC	iiiD
iv	$4^3$ balls	ivA	ivB	ivC	ivD
v	$8^3$ balls	vA	vB	vC	vD



# Simulation Results $M=0.9$

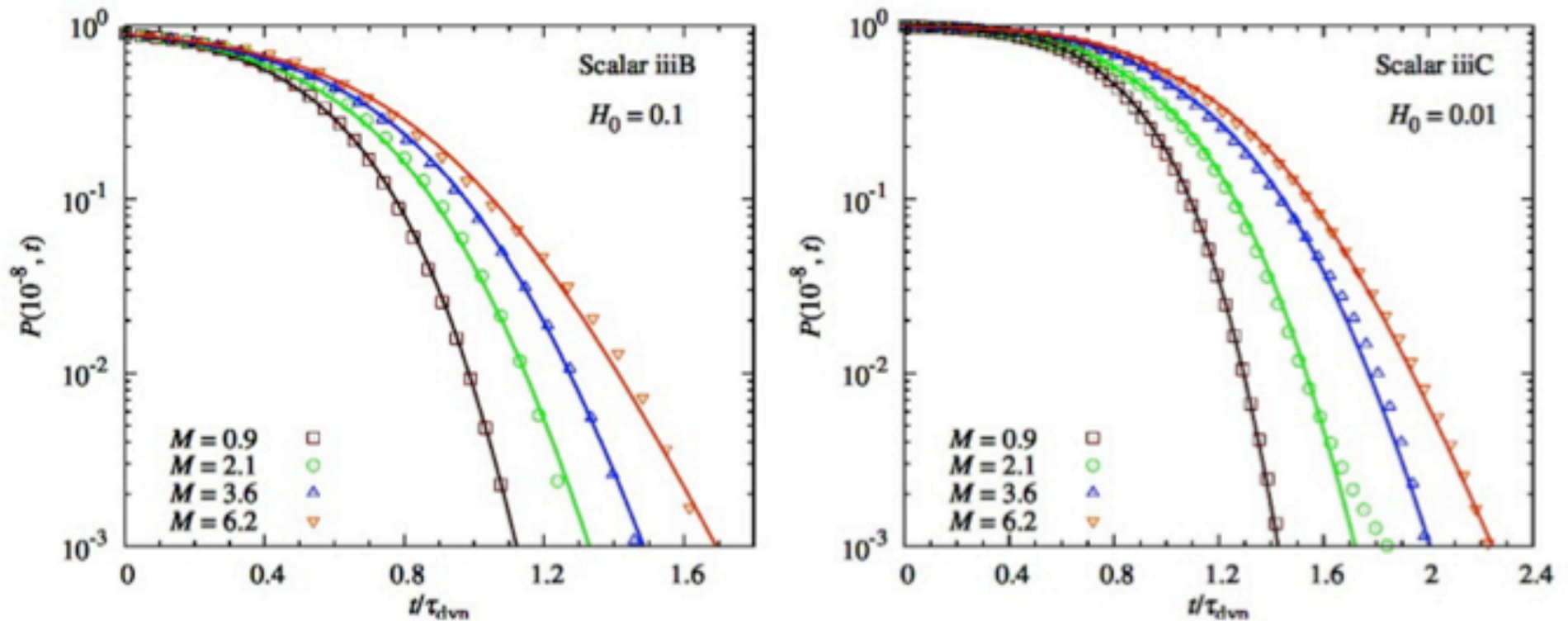


# Simulation Results $M=6.2$



Pan, ES, & Scalo (2012,2013)

# Evolution



**Extremely well fit by generalized convolution model**

$$\frac{dP}{dt} = - \frac{n_s}{\tau_{scon}} P(1 - P^{1/n_s})$$

## We fit it all with 2 parameters

$$\tau_{\text{con1}} = [0.225 - 0.055 \exp(-M^{3/2}/4)] \\ \times \left(\frac{L_p}{L_f}\right)^{0.63} \left(\frac{Z_c}{10^{-7}\langle Z \rangle}\right)^{0.015}, \quad \text{if } P \geq 0.9$$

$$\tau_{\text{con2}} = [0.335 - 0.095 \exp(-M^2/4)] \quad \text{if } P < 0.9 \\ \times \left(\frac{L_p}{L_f}\right)^{0.63} \left(\frac{Z_c}{10^{-7}\langle Z \rangle}\right)^{0.02}, \quad \text{and}$$

$$n = 1 + 11 \exp(-M/3.5) \left(\frac{L_p}{L_f}\right)^{1.3},$$

## We fit it all with 2 parameters

$$\tau_{\text{con1}} = \left[ 0.225 - 0.055 \exp(-M^{3/2}/4) \right] \text{ if } P \geq 0.9$$

$$\tau_{\text{con2}} = \left[ 0.335 - 0.095 \exp(-M^2/4) \right] \text{ if } P < 0.9$$

$$n = 1 + 11 \exp(-M/3.5)$$

$$\mathbf{v}_T \approx \Delta \mathbf{x} \frac{|\mathbf{d}_i \mathbf{v}_j + \mathbf{d}_j \mathbf{v}_i|}{2}$$

2

Smagorinsky (1963)

## Subgrid Model for Evolution Primordial Fraction

$$\frac{D(\rho P)}{Dt} = - \frac{n_s \rho}{\tau_{\text{scon}}} P (1 - P^{1/n_s}) - \dot{\rho}_{\text{ejecta}} P$$

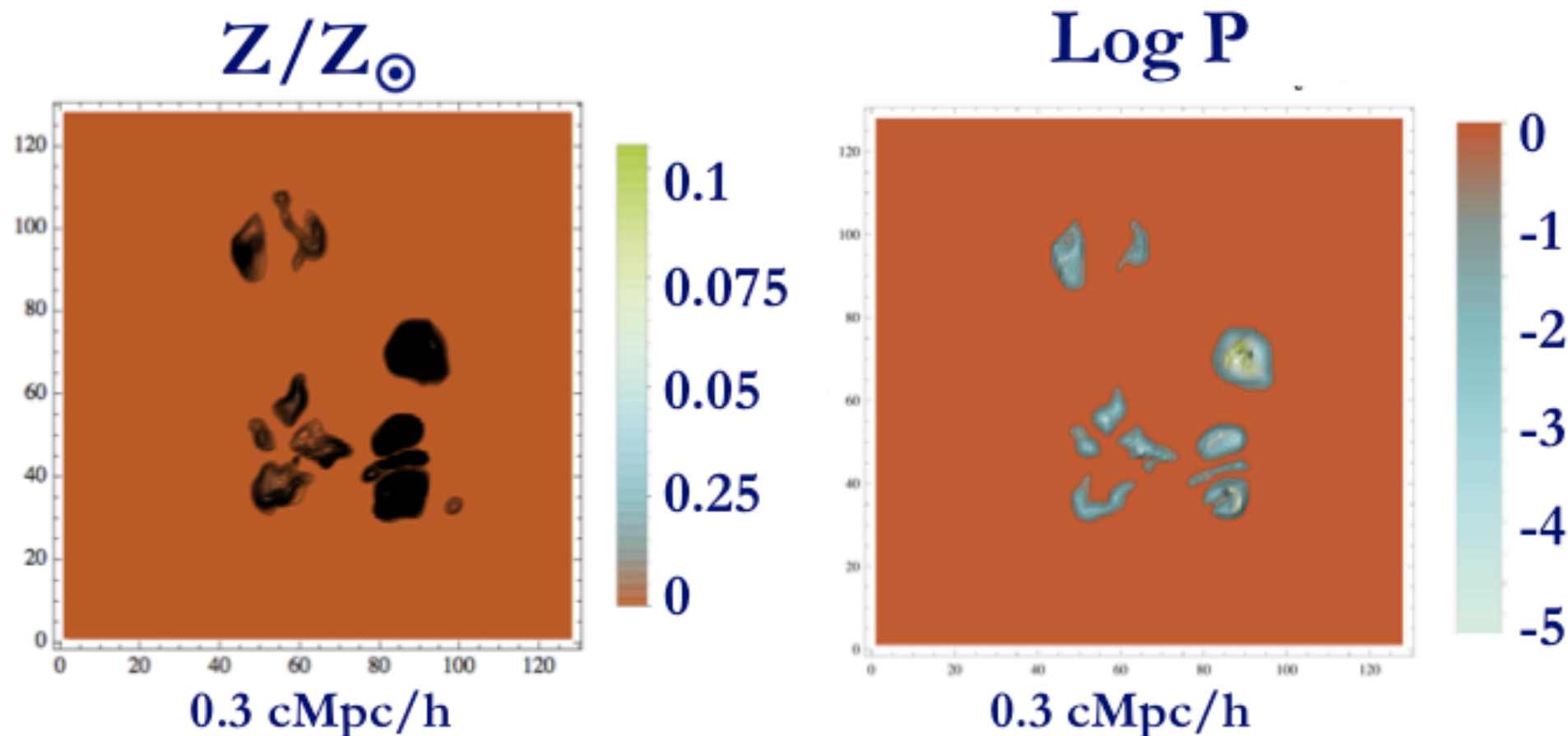
$P$  - Primordial Fraction

$\rho$  - Density

$\dot{\rho}_{\text{ejecta}}$  - Rate at which ejecta is being added to a cell

$n_s, \tau_{\text{scon}}$  - Fit functions to local turbulent Mach number and  $Z/Z_c$  provided in Pan, ES, & Scalo (2013)

# Evolution of Primordial Fraction (Test run @ $z=9$ )



We are implementing this now into the RAMSES code.

with R. Sarmiento, ES

# Thanks!

If you can track metals  
in your simulation (or  
even semi-analytical  
model), you can track  
primordial fraction!



Primordial Fraction