High performance computing and numerical modeling

Volker Springel

Plan for my lectures

Lecture 1: Collisional and collisionless N-body dynamics

Lecture 2: Gravitational force calculation

Lecture 3: Basic gas dynamics

Lecture 4: Smoothed particle hydrodynamics

Lecture 5: Eulerian hydrodynamics

Lecture 6: Moving-mesh techniques

Lecture 7: Towards high dynamic range

Lecture 8: Parallelization techniques and current computing trends

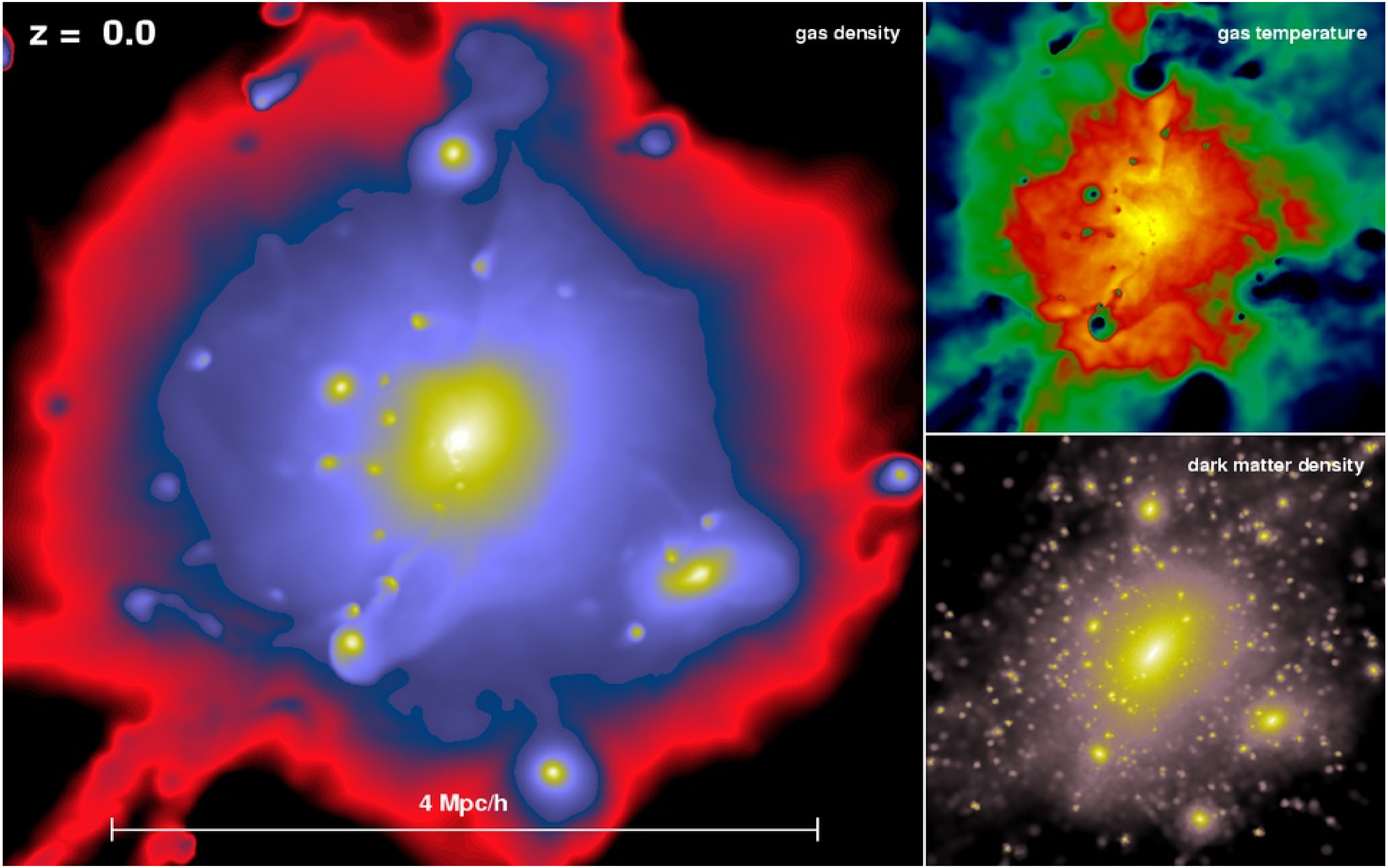
Heidelberg Institute for Theoretical Studies
HITS

Universität Heidelberg

43rd Saas Fee Course
Villars-Sur-Ollon, March 2013

Non-radiative gas shows markedly different behavior from dark matter once pressure forces become important

A SIMULATED CLUSTER WITH GAS



The Euler equations for inviscid gas dynamics

LAGRANGIAN FORM

Convective derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

Equation of motion:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho}$$

Continuity equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot \mathbf{v} = 0$$

Thermal energy equation:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{\rho} \nabla \cdot \mathbf{v}$$

Equation of state:

$$P = (\gamma - 1)\rho u \qquad \gamma = \frac{c_P}{c_v}$$

For mono-atomic gas: $\gamma = \frac{5}{3} \qquad \mu\, u = \frac{3}{2} k_B T$

Entropy equation:

$$\frac{\mathrm{d}A}{\mathrm{d}t} = 0 \qquad A \equiv \frac{P}{\rho^\gamma}$$

The Euler equations for inviscid gas dynamics

EULERIAN FORM

Mass conservation:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0$$

Momentum conservation:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v}\mathbf{v}^T + P) = 0$$

Energy conservation:

$$\frac{\partial}{\partial t}(\rho e) + \nabla[(\rho e + P)\mathbf{v}] = 0$$

Total specific energy:

$$e = \frac{1}{2}\mathbf{v}^2 + u$$

The Navier-Stokes equations for viscous fluids

FLOW WITH FINITE VISCOSITY

mass conservation: $$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0$$

momentum conservation: $$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v}\mathbf{v}^T + P) = \nabla \mathbf{\Pi}$$

energy conservation: $$\frac{\partial}{\partial t}(\rho e) + \nabla[(\rho e + P)\mathbf{v}] = \nabla(\mathbf{\Pi}\mathbf{v})$$

Viscous stress tensor:

$$\mathbf{\Pi} = \eta \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3}(\nabla \cdot \mathbf{v})\mathbf{1}\right] + \xi(\nabla \cdot \mathbf{v})\mathbf{1}$$

Special case: incompressible flow

Kinematic viscosity: $$\nu \equiv \frac{\eta}{\rho}$$

$$\frac{D\mathbf{v}}{Dt} = -\frac{\nabla P}{\rho} + \nu \nabla^2 \mathbf{v}$$

The equations of ideal magneto-hydrodynamics (MHD)

FLOW OF PERFECTLY CONDUCTING MEDIA

$\sigma = \infty$ from Ohm's law: $\mathbf{j} = \sigma \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \longrightarrow \mathbf{E} = -\frac{\mathbf{v} \times \mathbf{B}}{c}$

only magnetic field left in Maxwell's equations:

Induction equation: $$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) = 0$$

Divergence constraint: $$\nabla \cdot \mathbf{B} = 0$$

changes in the Euler equations:

$$P_{\rm tot} = P_{\rm gas} + \frac{1}{2}\mathbf{B}^2$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + P) = 0$$

$$e = u + \frac{1}{2}\mathbf{v}^2 + \frac{1}{2}\frac{\mathbf{B}^2}{\rho}$$

$$\frac{\partial}{\partial t}(\rho e) + \nabla[(\rho e + P)\mathbf{v} - \mathbf{B}(\mathbf{B} \cdot \mathbf{v}] = 0$$

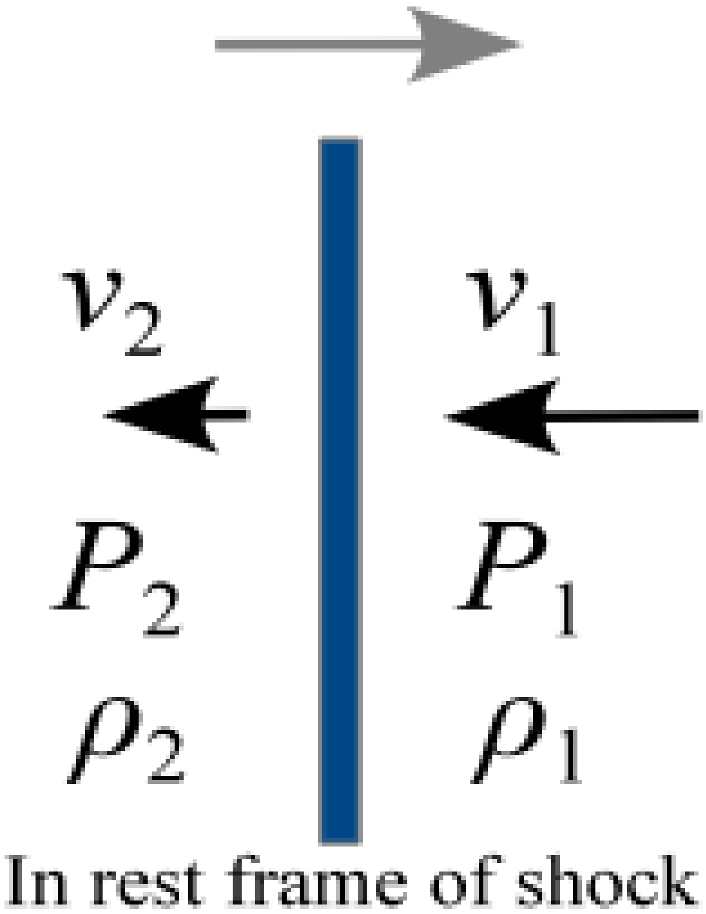
Shocks

The flow of an ideal gas can develop discontinuities, e.g. by sound wave steepening or by supersonically converging flows.

At such discontinuities, the entropy is no longer preserved.

The generation of the entropy happens in a thin shock layer where the viscosity can not be neglected any more.

Mach number: $\mathcal{M} = \frac{v_1}{c_1}$



The continuity of mass, energy and momentum flux across a shock relates the upstream and downstream flows.

Rankine-Huigonot jump conditions

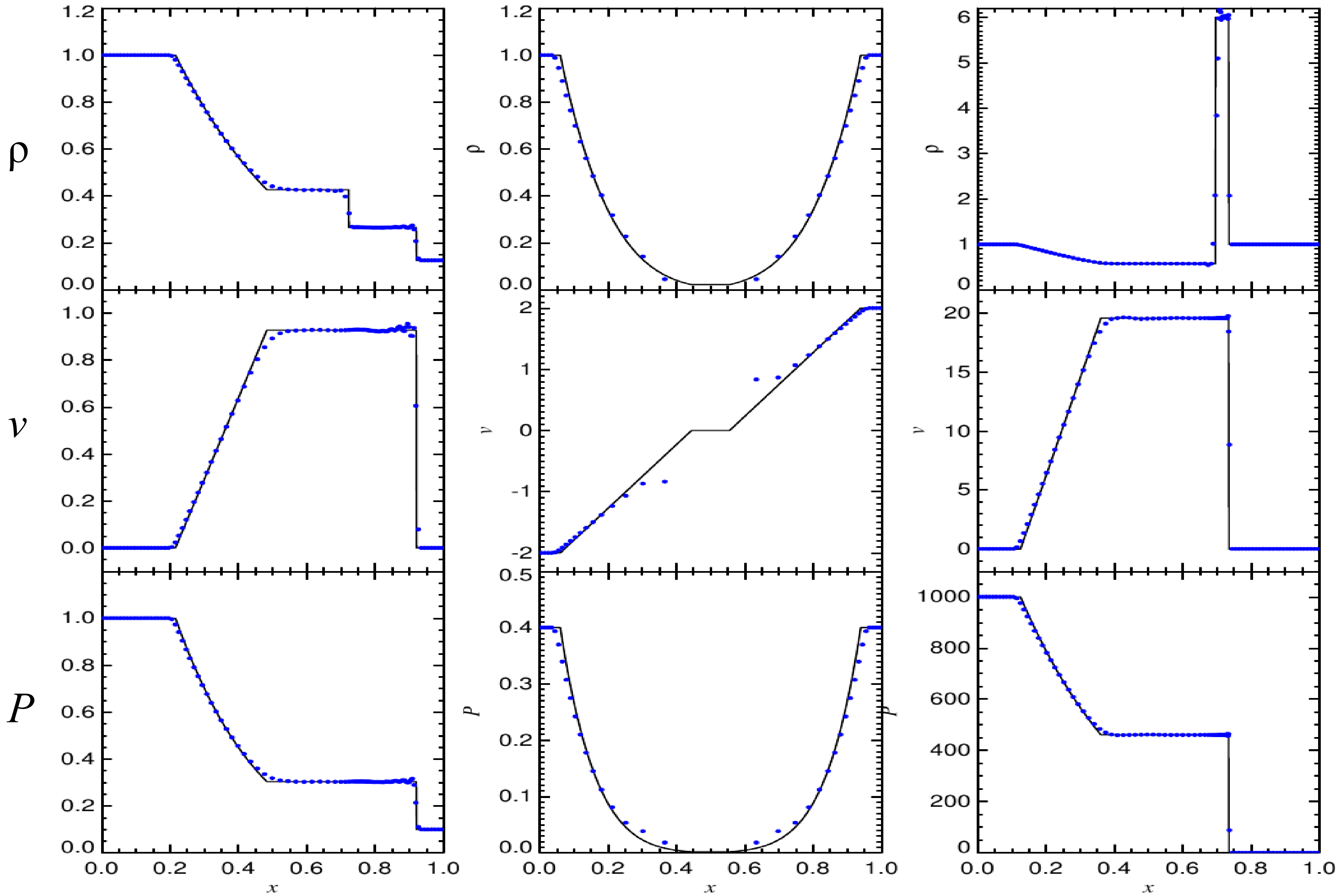
$$\frac{\rho_1}{\rho_2} = \frac{v_2}{v_1} = \frac{\gamma - 1}{\gamma + 1} + \frac{2}{(\gamma + 1)\mathcal{M}^2}$$

$$\frac{P_2}{P_1} = \frac{2\gamma\mathcal{M}^2}{\gamma + 1} - \frac{\gamma - 1}{\gamma + 1}$$

Note: density and velocity jumps are bound,
while the pressure and temperature jumps can be arbitrarily large.

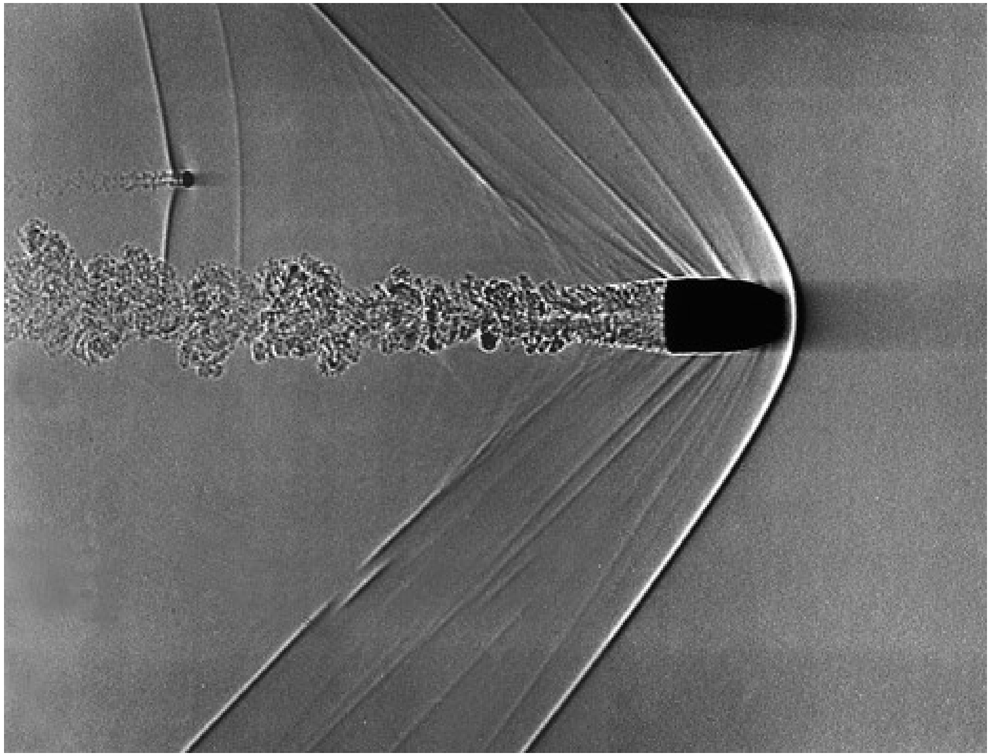
Sod-Shock tubes are simple test problems for shocks and rarefaction waves

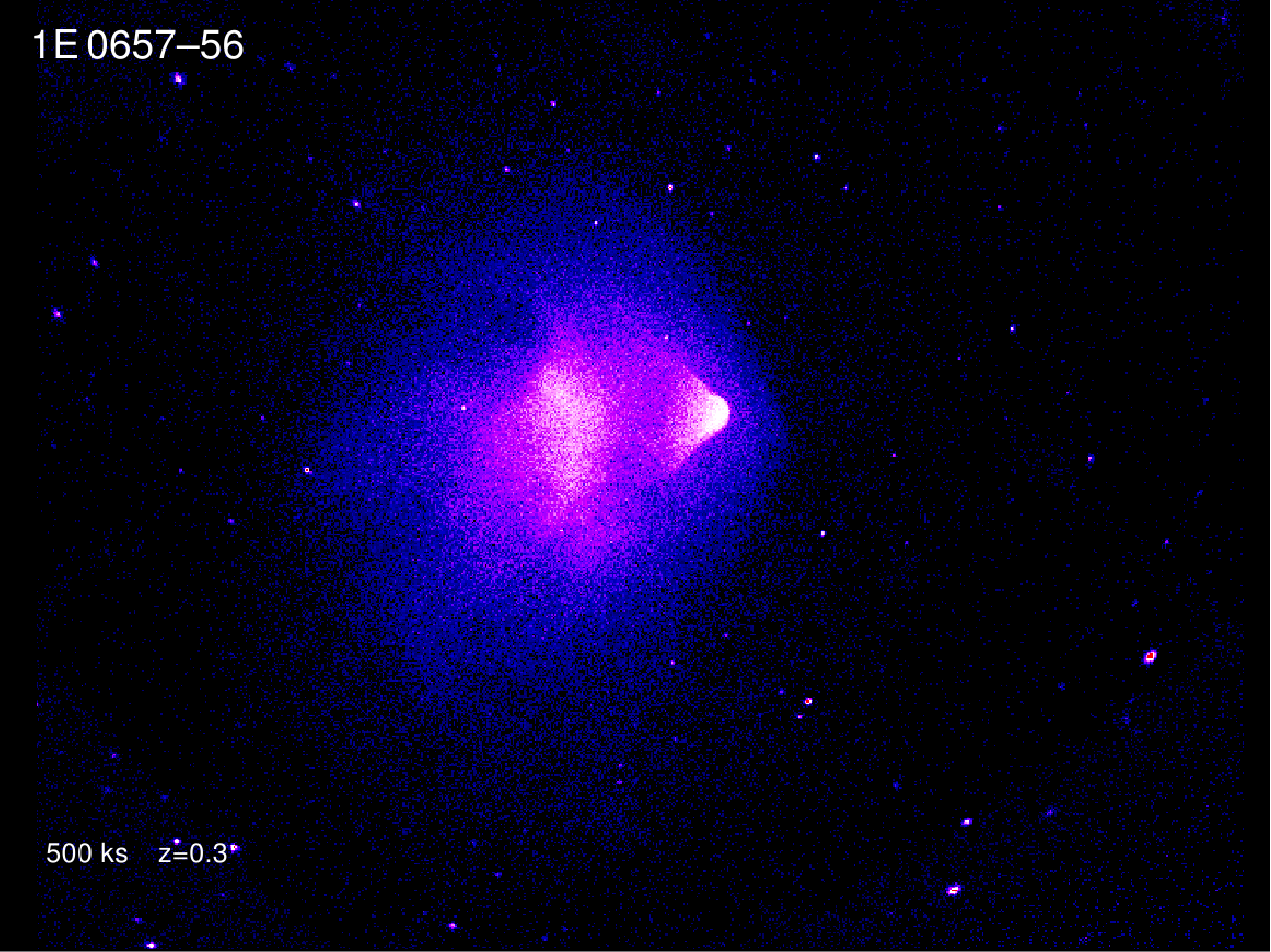
TWO SHOCK PROBLEMS AND A STRONG RAREFACTION



Supersonic motion creates shock waves

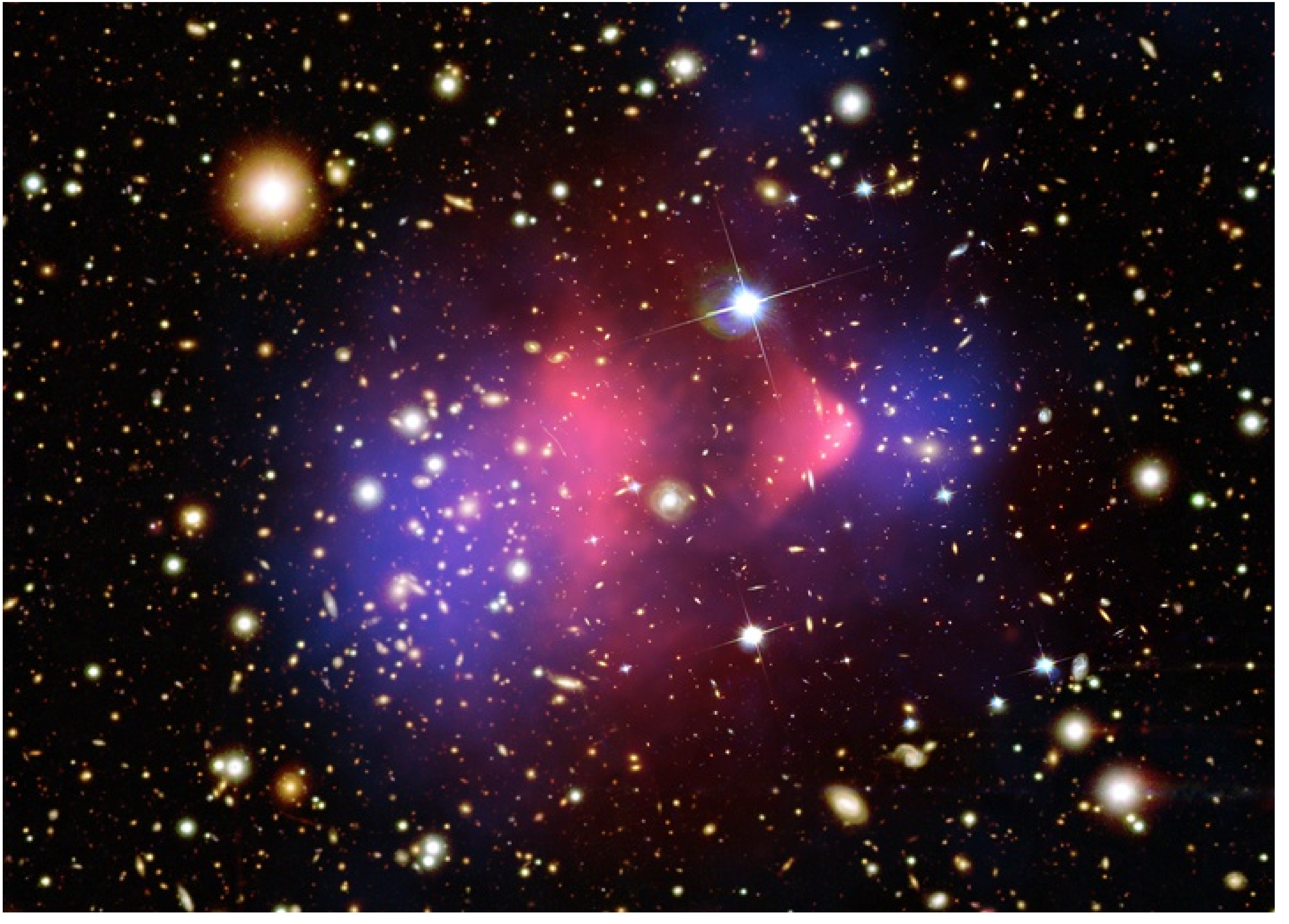
SHOCK WAVES OF A BULLET TRAVELLING IN AIR




1E 0657–56
500 ks
z=0.3

NASA Press Release Aug 21, 2006:

1E 0657-56: NASA Finds Direct Proof of Dark Matter

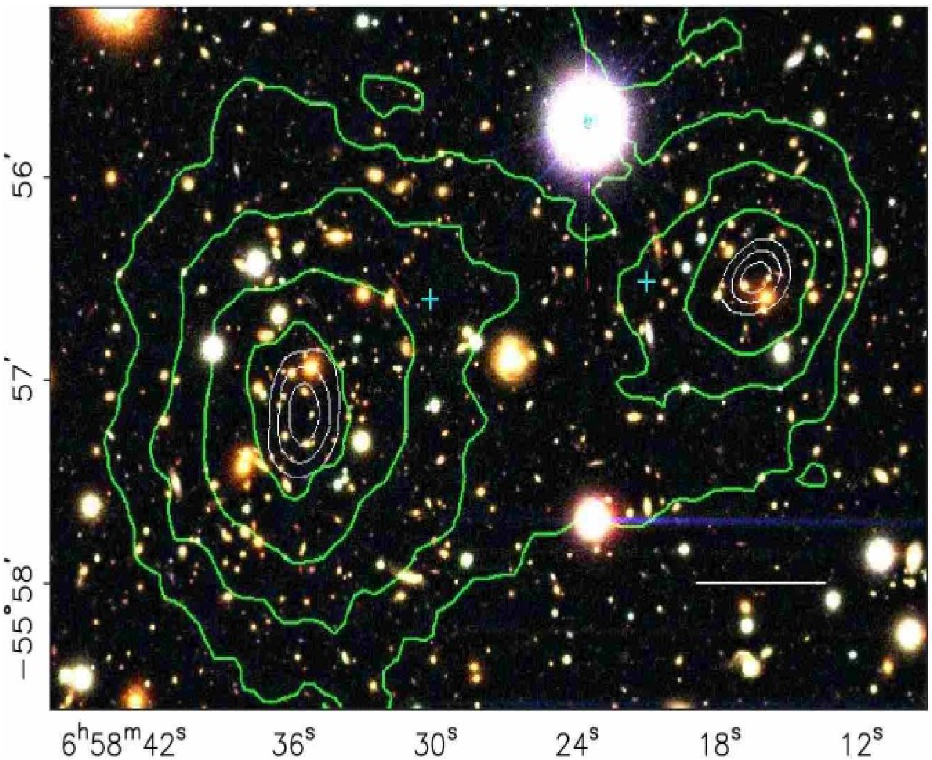


New weak lensing mass reconstructions have confirmed an offset between mass peaks and X-ray emission

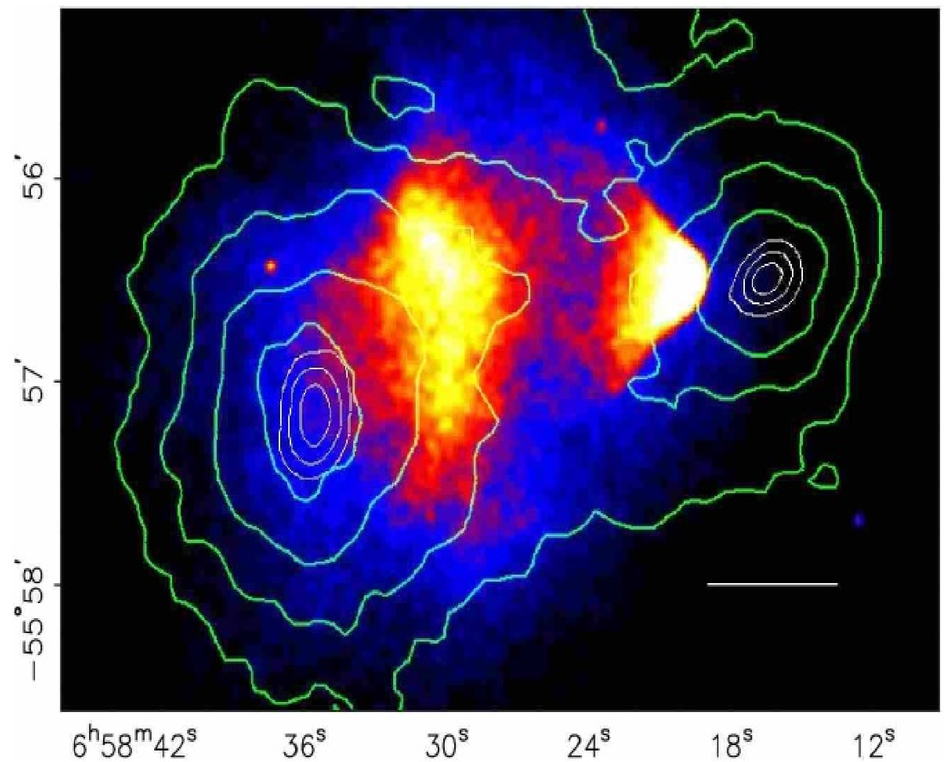
MASS CONTOURS FROM LENSING COMPARD TO X-RAY EMISSION

Clowe et al. (2006)

Magellan Optical Image



500 ksec Chandra exposure

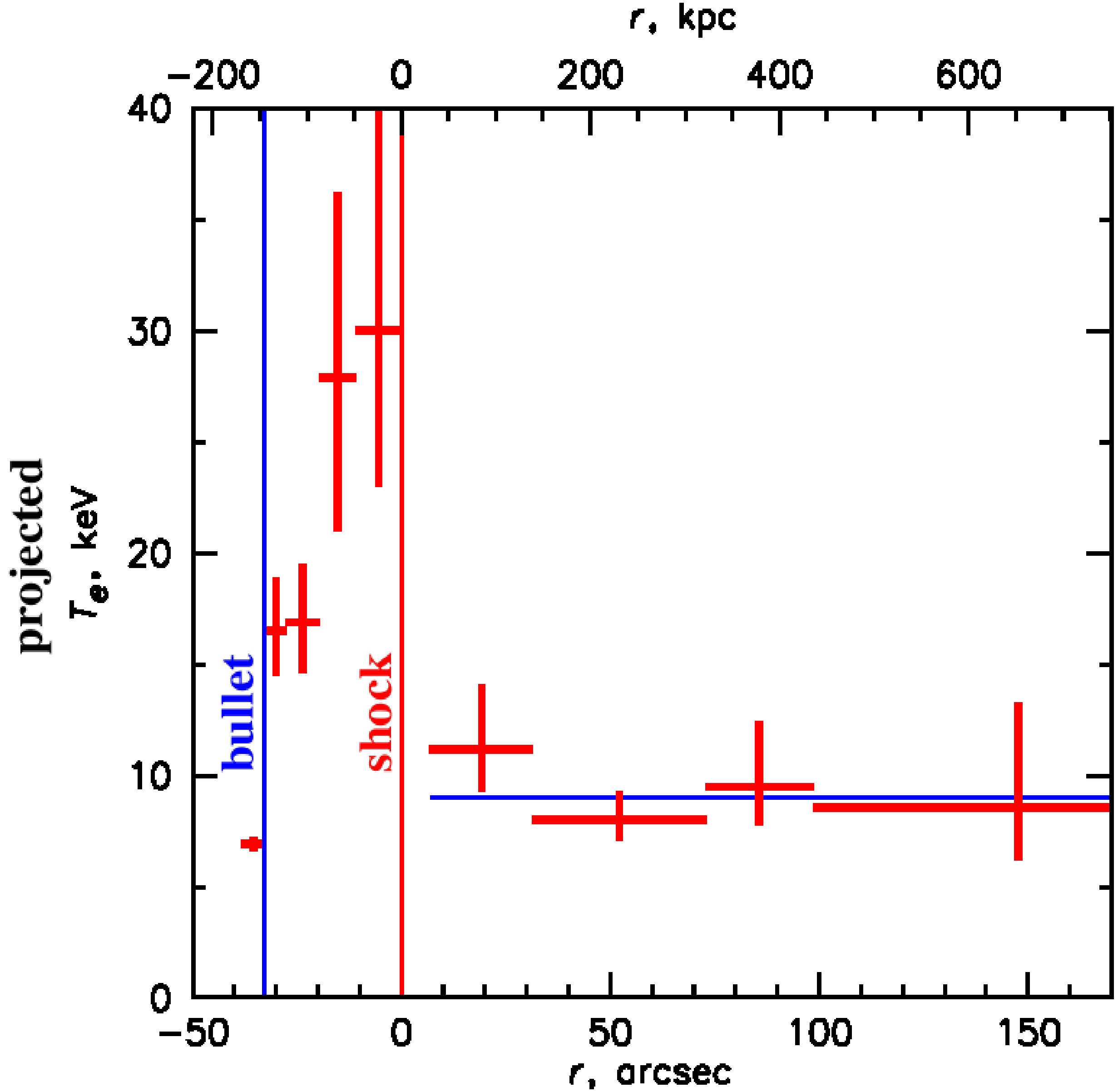


weak lensing mass contours overlaid

The temperature profile through the nose of the shock shows a strong shock and a cold front

X-RAY TEMPERATURE PROFILE FROM CHANDRA OBSERVATIONS

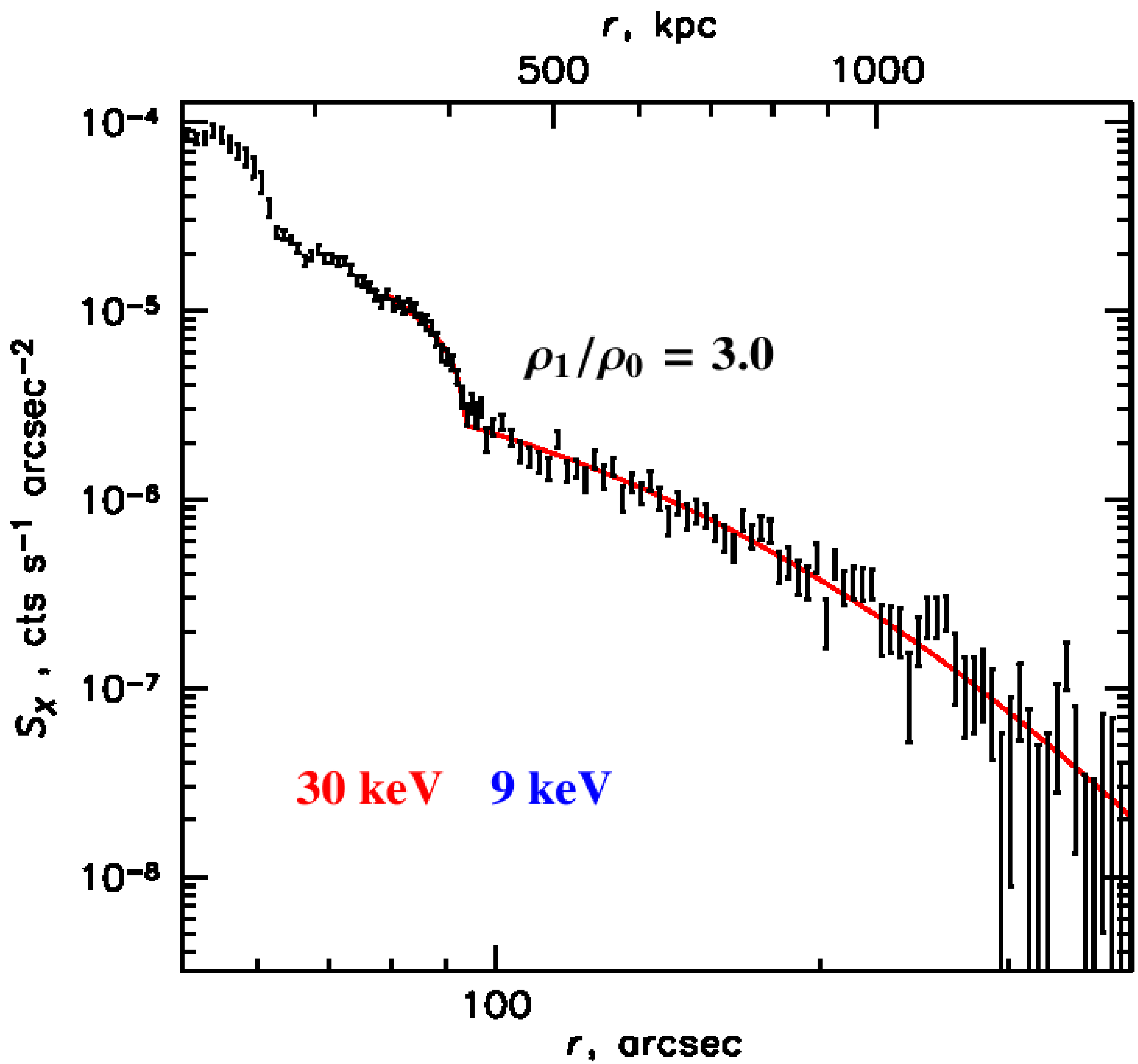
Markevitch et al. (2006)



Fitting the density jump in the X-ray surface brightness profile allows a measurement of the shock's Mach number

X-RAY SURFACE BRIGHTNESS PROFILE

Markevitch et al. (2006)



shock strength:

M = 3.0 ± 0.4

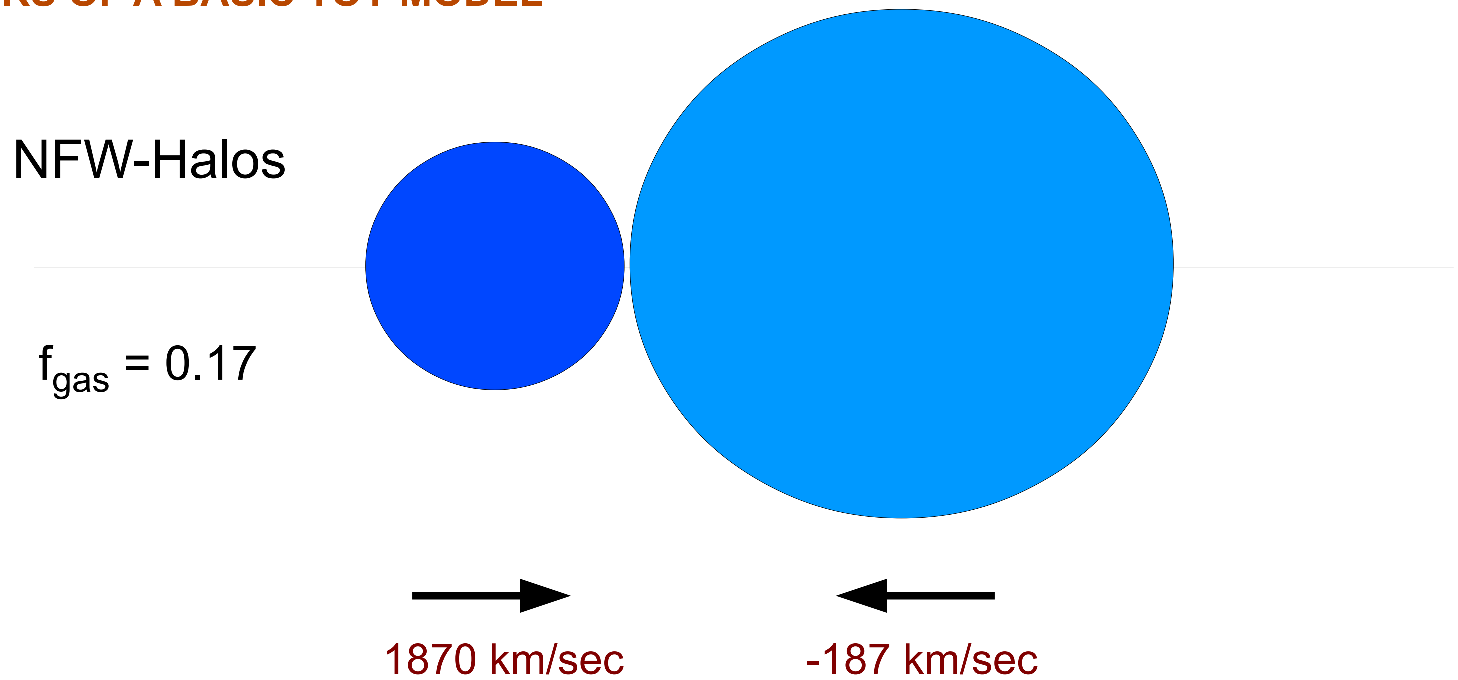
shock velocity:

***v_s* = 4700 km/s**

Usually, shock velocity has been identified with velocity of the bullet.

A simple toy merger model of two NFW halos on a zero-energy collision orbit

PARAMETERS OF A BASIC TOY MODEL



Mass model from **Clowe et al. (2006):**

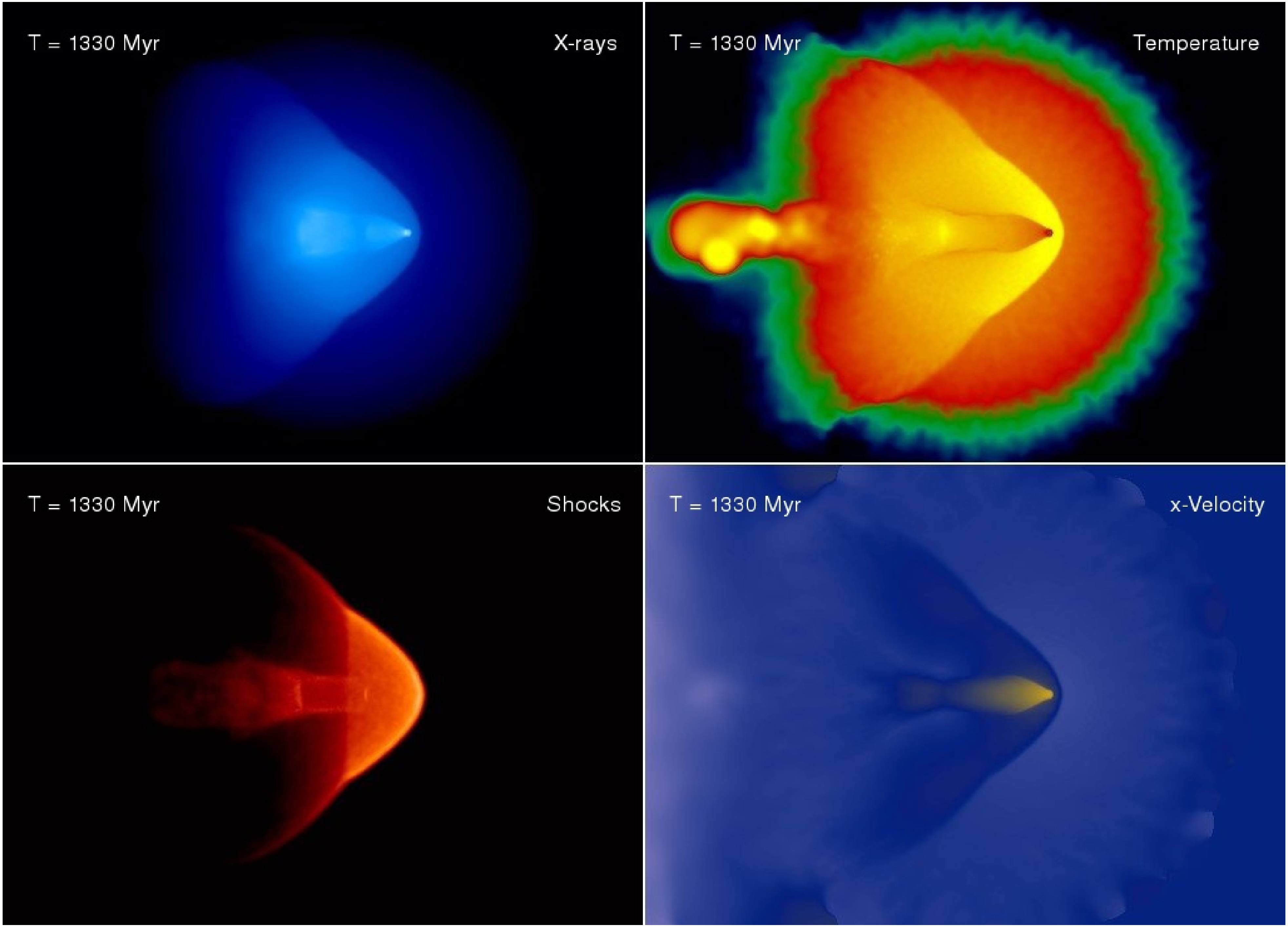
$\mathbf{M_{200} = 1.5 \times 10^{14}\ M_\odot}$

$R_{200} = 1.1$ Mpc
c = 7.2
V_{200} = 780 km/sec

$\mathbf{M_{200} = 1.5 \times 10^{15}\ M_\odot}$

$R_{200} = 2.3$ Mpc
c = 2.0
V_{200} = 1680 km/sec

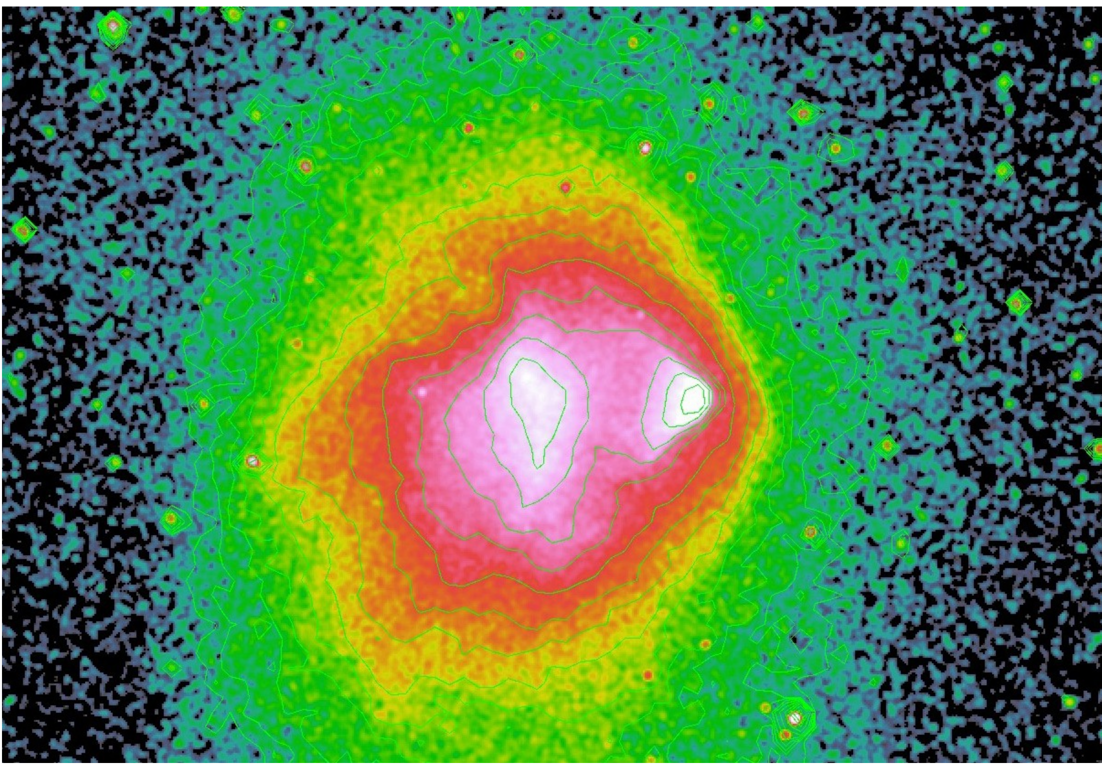
VIDEO OF THE TIME EVOLUTION OF A SIMPLE BULLET CLUSTER MODEL



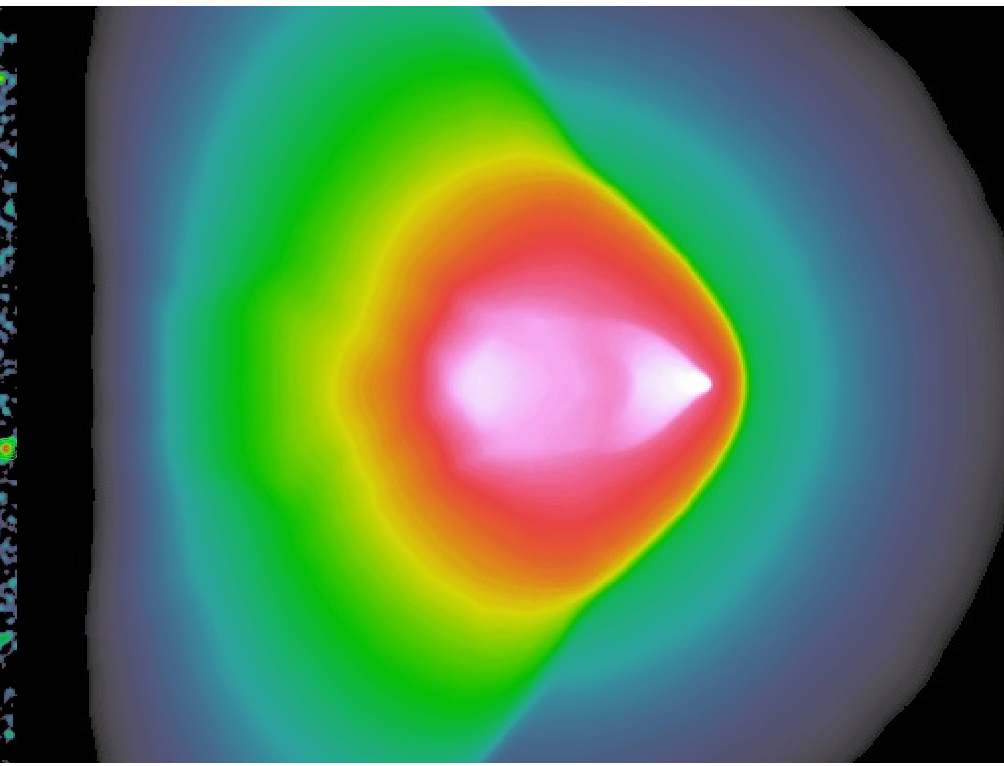
Drawing the observed X-ray map and the simulation images with the same color-scale simplifies the comparison

SIMULATED X-RAY MAP COMPARED TO OBSERVATION

Candra 500 ks image



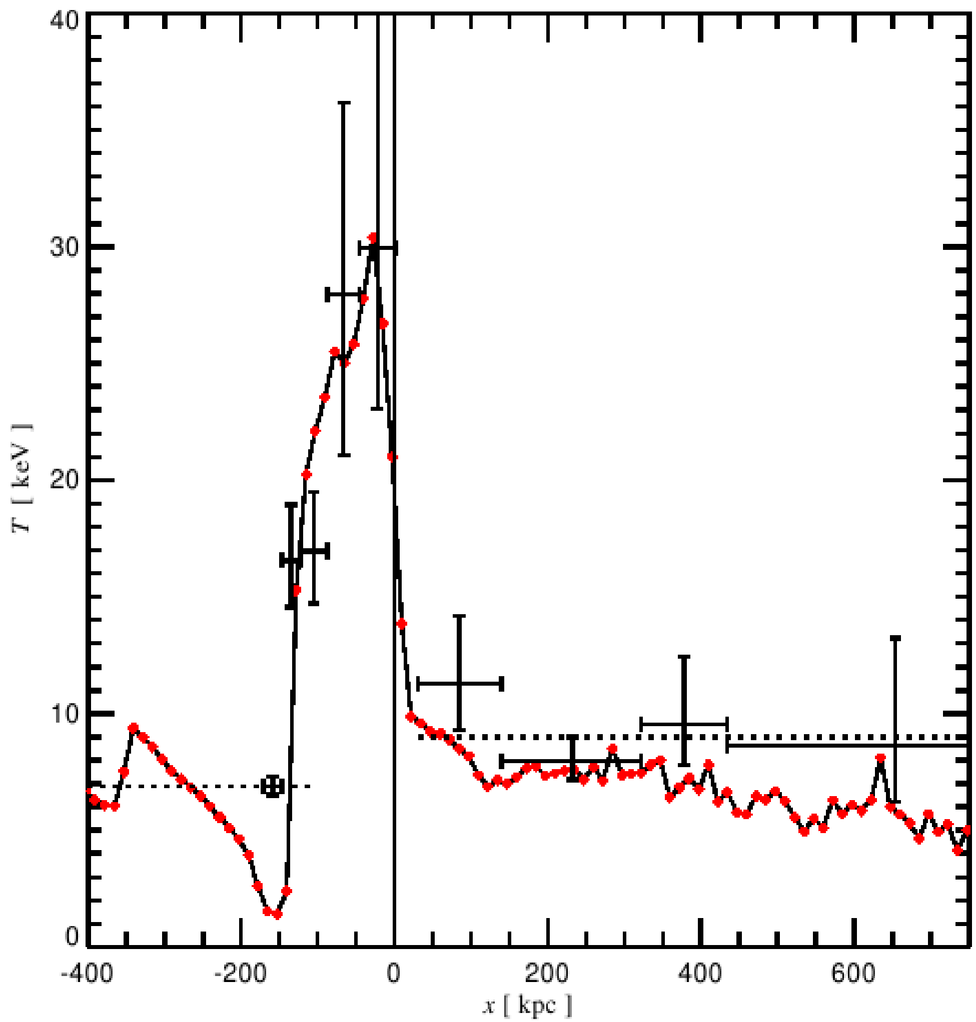
bullet cluster simulation



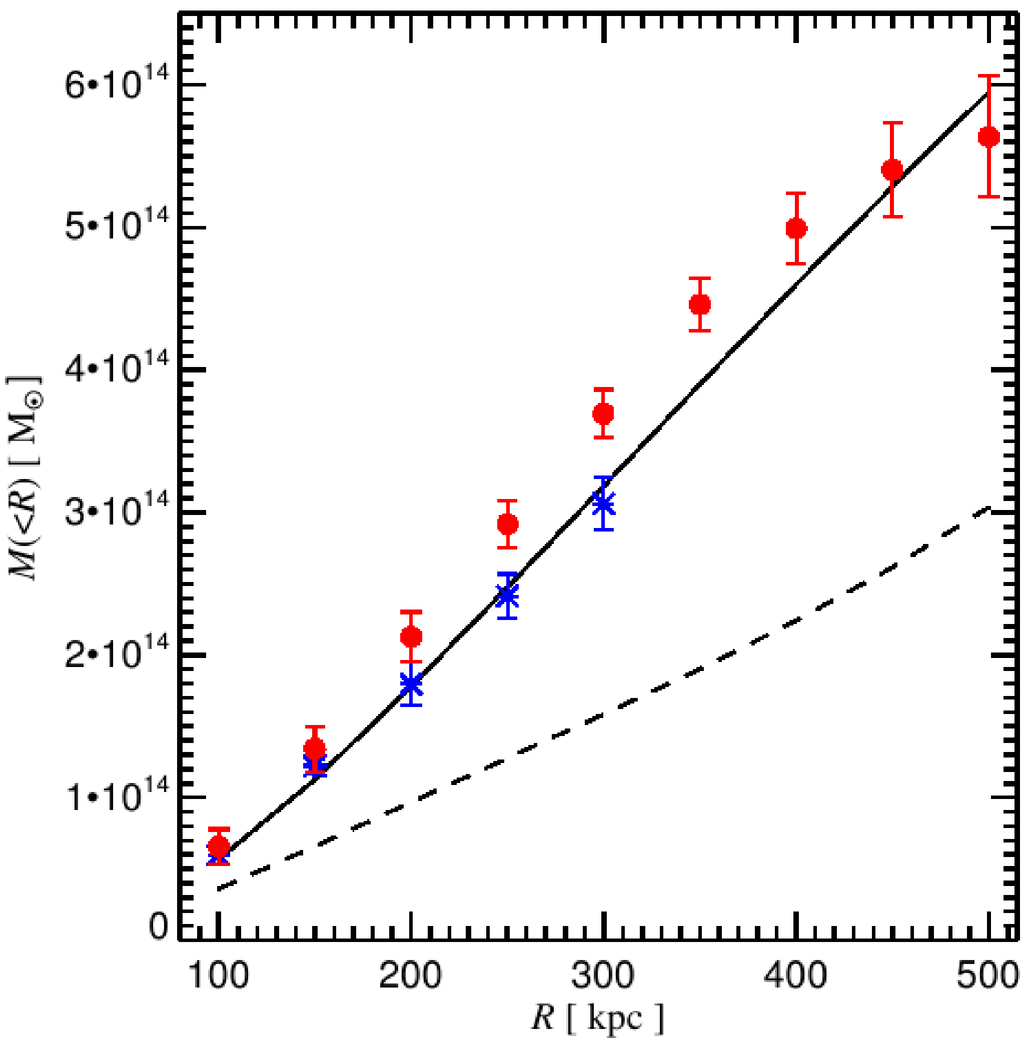
Springel & Farrar (2007)

The model also matches the observed temperature and mass profiles

COMPARISON OF SIMULATED TEMPERATURE AND MASS PROFILE WITH OBSERVATIONS



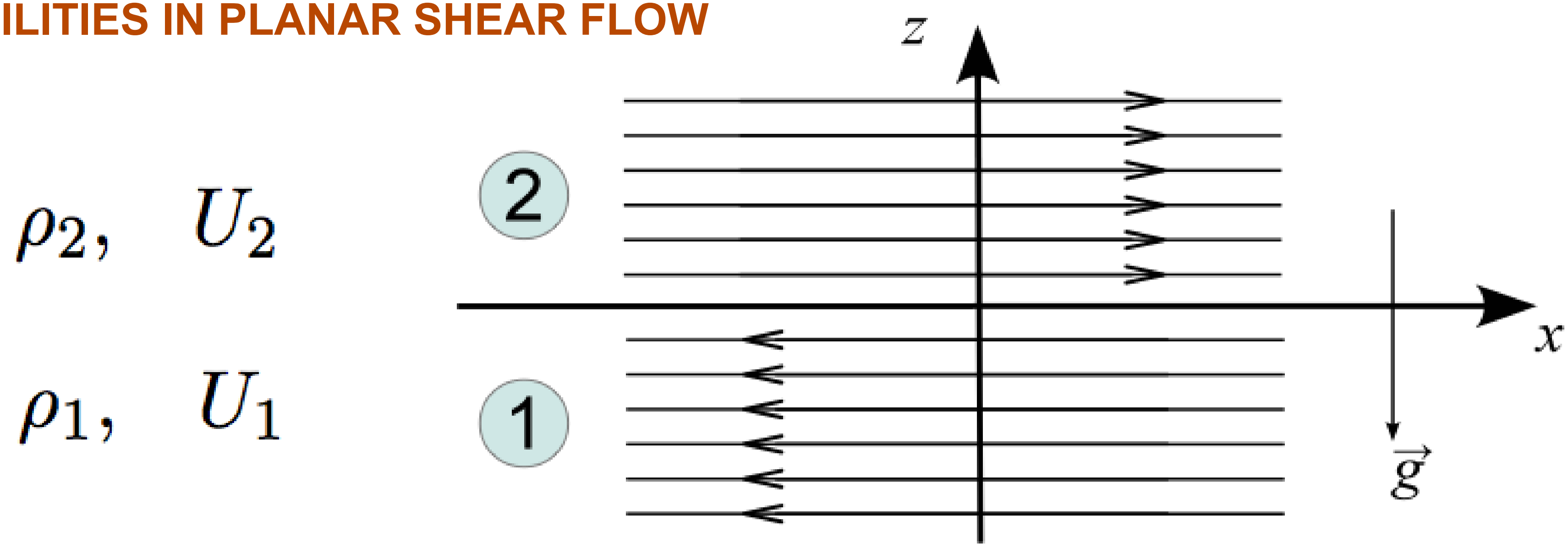
Data from **Markevitch et al. (2006)**



Data from **Bradac et al. (2006)**

In multidimensional hydrodynamics, interesting fluid instabilities can arise which can make a flow prone to develop turbulence

INSTABILITIES IN PLANAR SHEAR FLOW



Put in a wave-like perturbation at the interface and examine linear growth (eigemode analysis)

$$\phi_1 = \phi_1(z) \exp[i(kx - \omega t)]$$

Dispersion relation:

$$\omega^2(\rho_1 + \rho 2) - 2\omega k(\rho_1 U_1 + \rho_2 U_2) + k^2(\rho_1 U_1^2 + \rho_2 U_2^2) + (\rho_2 - \rho 1)kg = 0$$

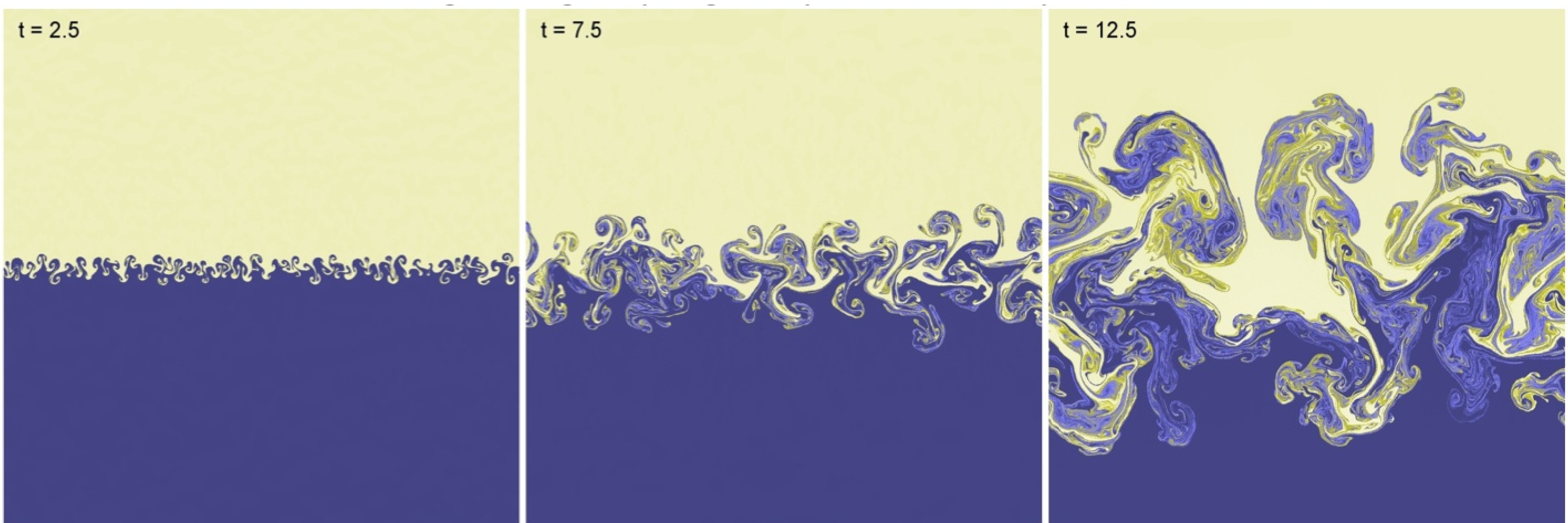
Rayleigh-Taylor instability

If there is no shear flow initially and only buoyancy, we get the RT instability

$$U_1 = U_2 = 0.$$

$$\omega^2 = \frac{(\rho_1 - \rho_2)kg}{\rho_1 + \rho_2}$$

Flow is stable if the lighter fluids is on top.



Kelvin-Helmholtz Instability

If there is no gravitational field, the shear flow is always unstable

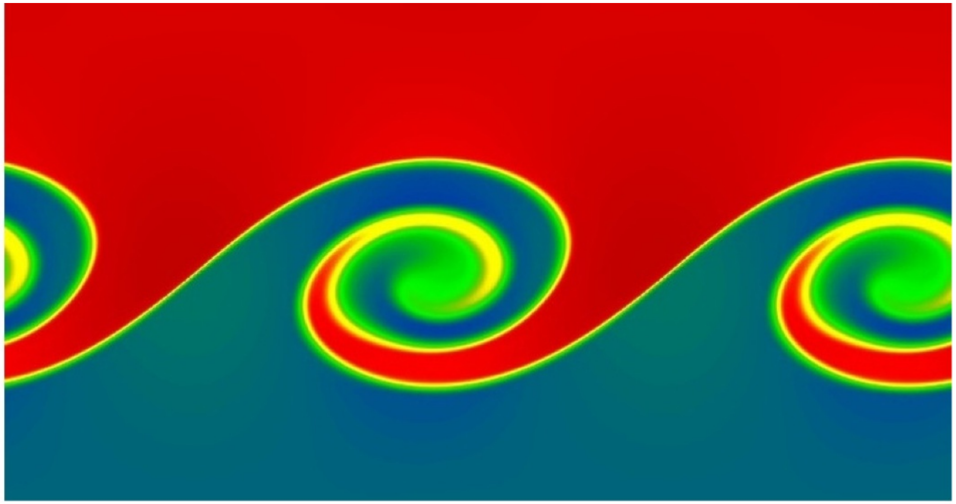
for $g = 0$ $$\omega_{1/2} = \frac{k(\rho_1 U_1 + \rho_2 U_2)}{\rho_1 + \rho_2} \pm i \frac{\sqrt{\rho_1 \rho_2}}{\rho_1 + \rho_2} |U_1 - U_2|$$

for $g > 0$ $$\omega = \frac{k(\rho_1 U_1 + \rho_2 U_2)}{\rho_1 + \rho_2} \pm \frac{\sqrt{-k^2 \rho_1 \rho_2 (U_1 - U_2)^2 - (\rho_1 + \rho_2)(\rho_2 - \rho_1) k g}}{\rho_1 + \rho_2}$$

Flow is stable if:

- Lighter fluid is on top
- Velocity difference is small enough

$$(U_1 - U_2)^2 < \frac{(\rho_1 + \rho_2)(\rho_1 + \rho_2) g}{k \rho_1 \rho_2}$$



Kelvin-Helmholtz instabilities seen in Nature