

High-Resolution RHD Simulations at Cosmological Scales with the GPU-Accelerated QUOKKA Code

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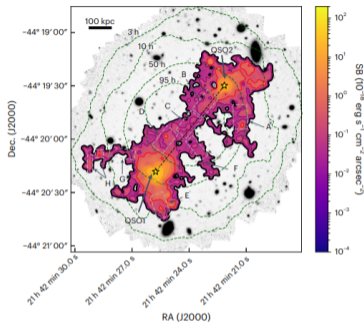
Preliminary results

Conclusion and perspectives

Introduction

Why Cosmology for Quokka?

- ▶ Recent advancements in observation of LSSs.
- ▶ Quokka is a state-of-art two-moment AMR RHD on GPUs.

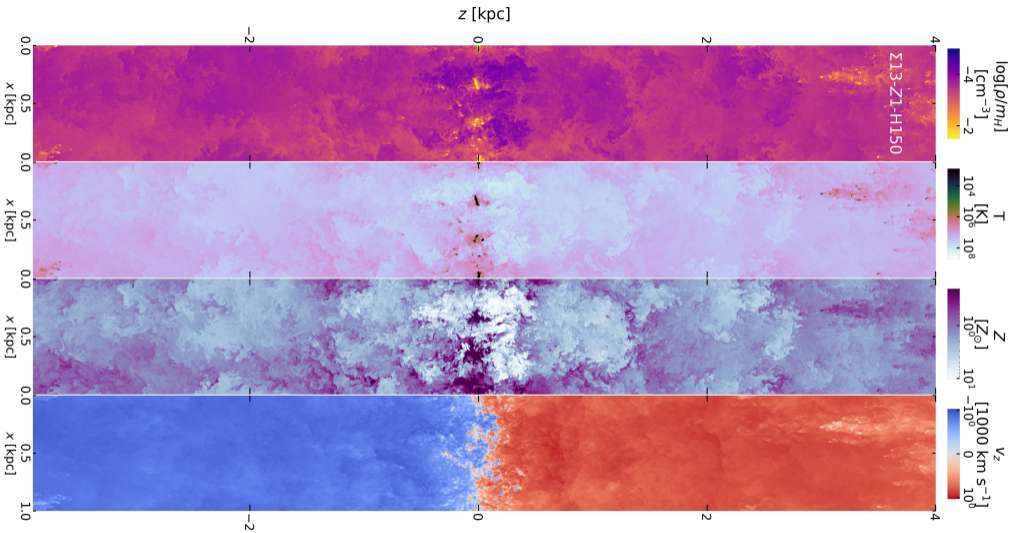


Quokka currently lacks a **cosmological module** to study LSSs.

Quokka is an AMReX-based two-moment **radiation hydrodynamics code** (which also includes self-gravity, particles, chemistry, and magnetic fields) optimized for **GPUs** and exploiting **MFF** (lab frame for radiation but comoving for matter), that uses the piecewise-parabolic method, with **AMR** and sub-cycling in time.



Quokka riding a rocket
(from the Quokka documentation).



Quokka in a nutshell

▶ **Radiative transfer:**

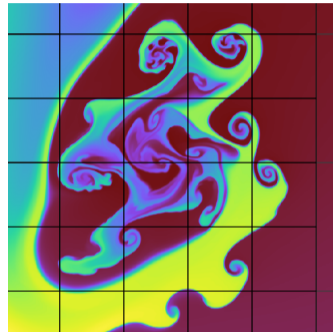
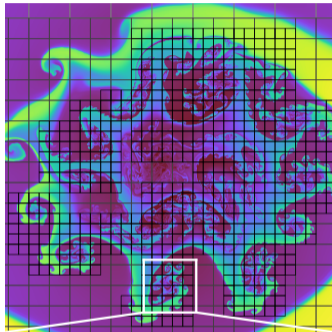
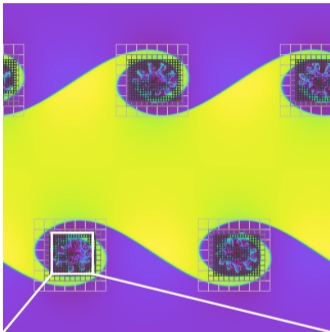
$$\frac{1}{c} \frac{\partial}{\partial t} I_\nu + \hat{\mathbf{n}} \cdot \nabla I_\nu = \eta_\nu - \kappa_\nu^{(\text{tot})} \rho I_\nu + \frac{1}{4\pi} \int \kappa_\nu^{(\text{sca})} \rho I_\nu d\Omega.$$

▶ **Operator split approach:**

1. **Hydro** (explicit, method-of-lines, PPM).
2. **Multigroup radiation** (explicit, MoL, two-moments, Levermore closure as default, RSLA).
3. **Local coupling** terms (implicit method: energy source terms \rightarrow momenta \rightarrow radiation work on the gas).

▶ **Sub-cycling in time:** flux register and $N_{\text{sub,max}} = 10$.

AMR



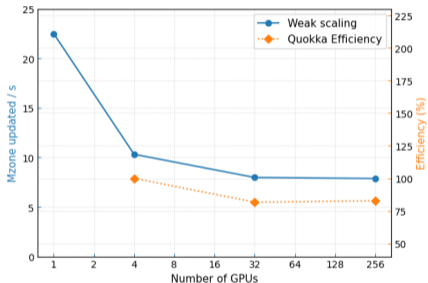
Still to be tested for cosmology!

Wibking & Krumholz (2022)

GPU scaling

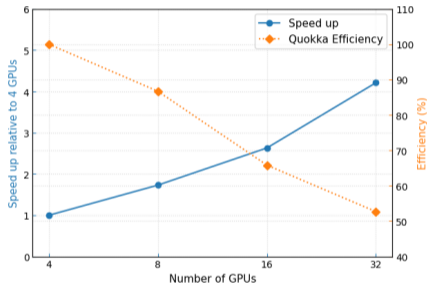
RHD test scaling on Gadi supercomputer at the National Computational Infrastructure (2 24-core Intel Xeon Platinum 8268 (Cascade Lake) 2.9 GHz CPUs and 4 Nvidia Tesla Volta V100-SXM2-32GB GPUs per node).

Weak scaling on GPU



Weak scaling: fixed number of computational cells per GPU.

Strong scaling on GPU

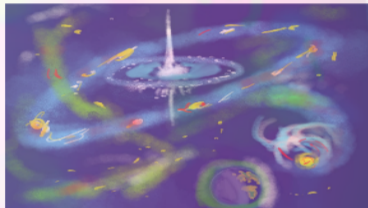
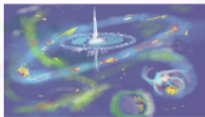


Strong scaling: minimize total runtime or total node-hours.

Still to be tested for cosmology!

Methods: the implementation

Cosmology for Quokka



Modular approach: Cosmology.hpp

- ▶ Adaptive **RK12** evolution of the scale factor.

$$H^2(a) = H_0^2 \left[\Omega_{r,0} \left(\frac{a_0}{a}\right)^4 + \Omega_{m,0} \left(\frac{a_0}{a}\right)^3 + \Omega_{k,0} \left(\frac{a_0}{a}\right)^2 + \Omega_{\Lambda,0} \right]$$

- ▶ **Hubble drag** and **adiabatic cooling** as geometrical source terms (analytical solutions).

$$p(a_{\text{new}}) = p_{\text{old}} \left(\frac{a_{\text{old}}}{a_{\text{new}}} \right) \quad e_{\text{int}}(a_{\text{new}}) = e_{\text{int,old}} \left(\frac{a_{\text{old}}}{a_{\text{new}}} \right)^{3(\gamma-1)}$$

- ▶ **Second order accuracy** via Strang splitting coupling of hydro with Cosmology.hpp source terms and $a(t)$ updated at midpoint and end of hydro timestep.

Cosmology integration for hydro

- ▶ **CFL** signal velocity rescaling

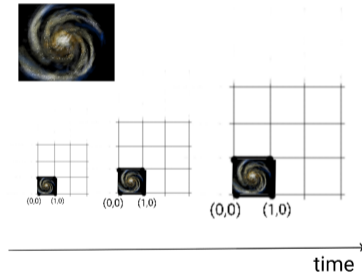
$$v_{\text{comov}} = v_{\text{phys}}/a.$$

- ▶ Comoving **Poisson Gravity**

$$\nabla^2 \phi = \frac{4\pi G}{a} (\rho_c - \bar{\rho}_c).$$

- ▶ Comoving **Hydro Fluxes**:

$$\nabla_r = \nabla_x/a$$

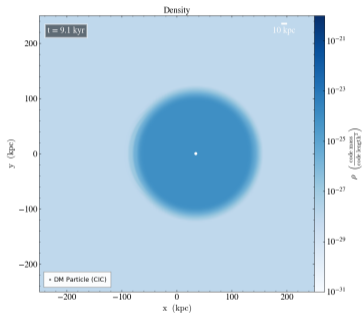


Cosmology for particles

Strang-split approach, interleaving the universe expansion with the previous **KDK** leapfrog scheme:

1. **Pre-Kick Hubble Drag:** $v_n \rightarrow v_n^* = v_n \cdot (a_n/a_{n+1/2})$
2. **First gravitational half-kick:** $v_n^* \rightarrow v_{n+1/2} = v_n^* + \frac{\Delta t}{2} \cdot g_n/a_n$
3. **Midpoint Drift:** $x_{n+1} = x_n + \Delta t \cdot v_{n+1/2}/a_{n+1/2}$
4. **Second gravitational half-kick:** $v_{n+1/2} \rightarrow v_{n+1}^{**} = v_{n+1/2} + \frac{\Delta t}{2} \cdot g_{n+1}/a_{n+1}$
5. **Post-Kick Hubble Drag:** $v_{n+1}^{**} \rightarrow v_{n+1} = v_{n+1}^{**} \cdot (a_{n+1/2}/a_{n+1})$.

Mass deposition and CFL



Particle initialized in `testCosmoSphere.cpp`.

- ▶ **Particle CFL** condition

$$\Delta t \leq \text{CFL} \cdot \frac{a \cdot \Delta x}{|v_{\text{pec}}|}.$$

- ▶ **Scaling CIC** mass projection for Poisson

$$\text{RHS} = \frac{4\pi G}{a} \frac{m}{\Delta V}.$$

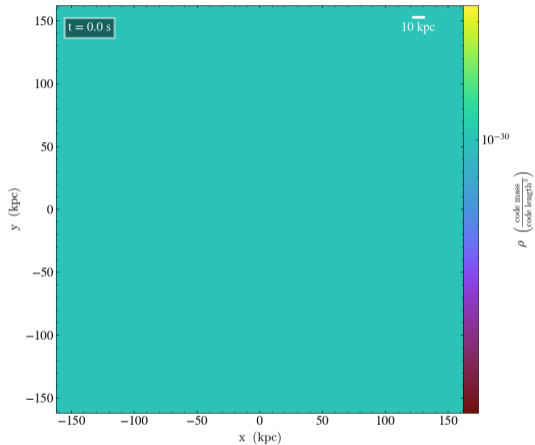
- ▶ **Particle drift**

$$x = \frac{v_{\text{pec}} \Delta t}{a}.$$

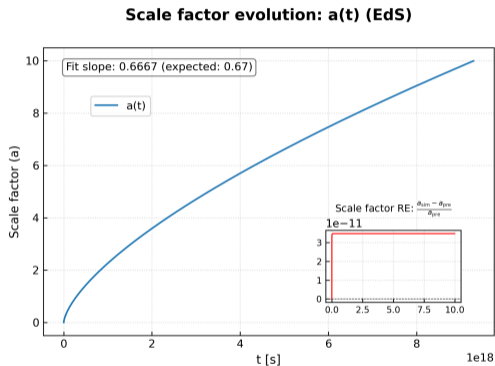
Tests and results

CosmoExpansion test

- ▶ **EdS homogeneous** universe filled by drifting ideal gas.
- ▶ **295 Gyr** cosmological evolution ($a_{\text{in}} = 10^{-3}$, $a_{\text{fin}} = 10$).
- ▶ Baseline test for **Friedmann solver** and **hydro**.



Scale factor validation



Analytical **EdS** solution

$$a(t) = \left(\frac{3}{2}H_0 t\right)^{2/3}.$$

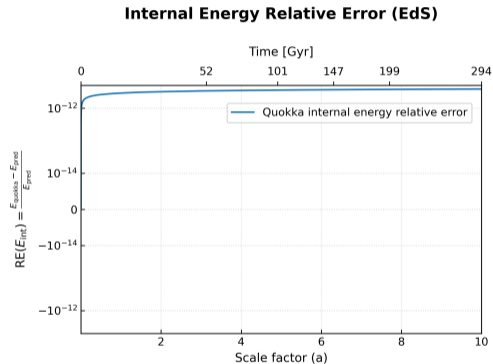
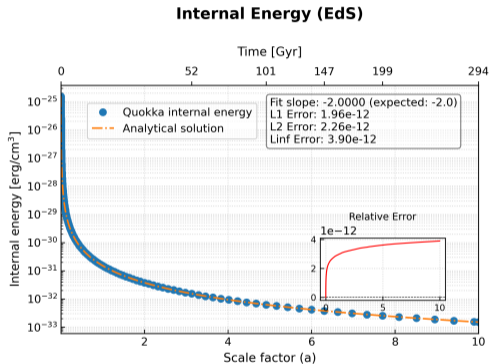
► Max **RE**

$$\max[|a_{\text{num}} - a_{\text{theo}}| / a_{\text{theo}}] = 3.47 \times 10^{-11}.$$

► Quokka **PL** fit vs analytical exponent:

$$\Delta\alpha = 9.53 \times 10^{-13}.$$

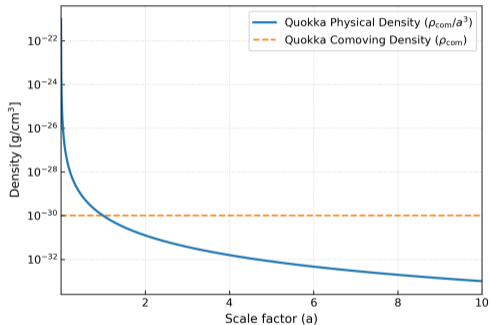
Internal energy: adiabatic cooling



$$e_{int}(a) = e_{int,0} \left(\frac{a_{init}}{a} \right)^{3(\gamma-1)}. \quad (1)$$

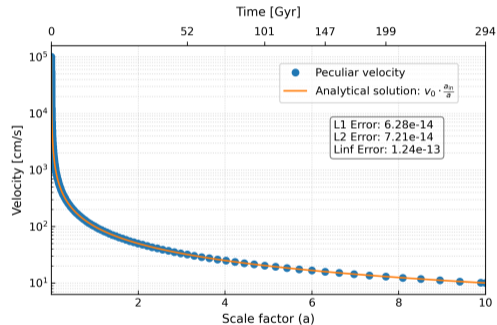
Density and Hubble drag

Physical vs comoving density (EdS)



$$\rho_{phys}(a) = \rho_{com} a^{-3}$$

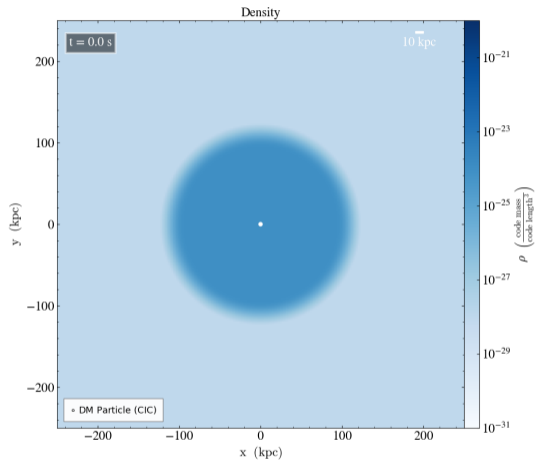
Peculiar Velocity Decay: Hubble Drag (EdS)



$$v_{phys}(a) = v_{com} a^{-1}$$

CosmoSphereDM test

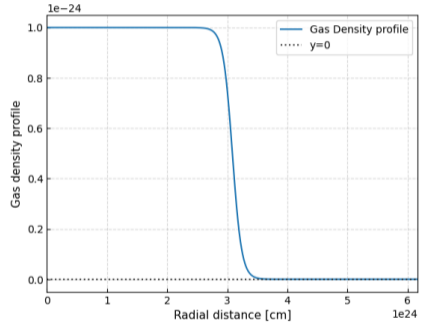
- ▶ **DM** particle centered on a **gas** sphere.
- ▶ **Same** drift **velocity** of 10^3 km/s for 10 Gyr.
- ▶ **Final shift** of 0.21 kpc (0.11 cells) after traveling 70.9 kpc.



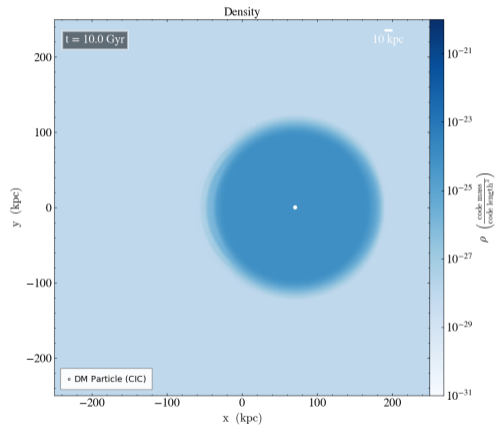
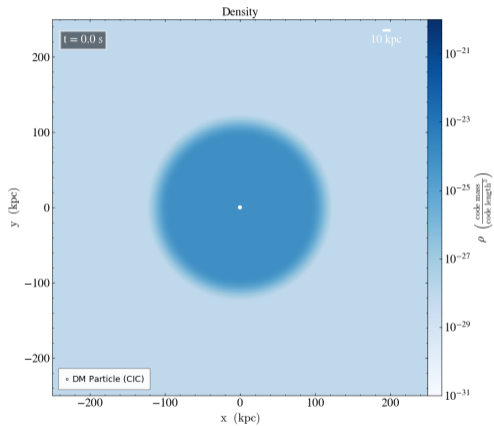
Gas density profile

- ▶ **Gas density profile** smoothed using a hyperbolic tangent transition.
- ▶ Gas **CoM** retrieved via weighted mean

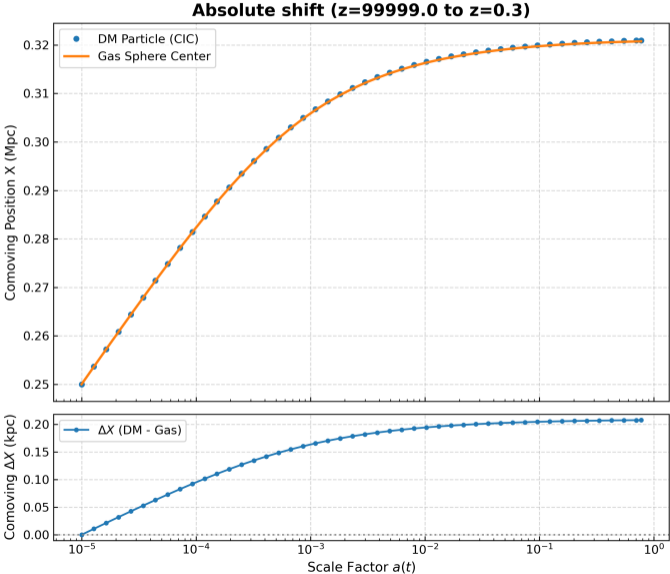
$$X_{\text{gas}} = \frac{\sum_{i,j,k} \rho_{i,j,k} \cdot X_{i,j,k}}{\sum_{i,j,k} \rho_{i,j,k}} .$$



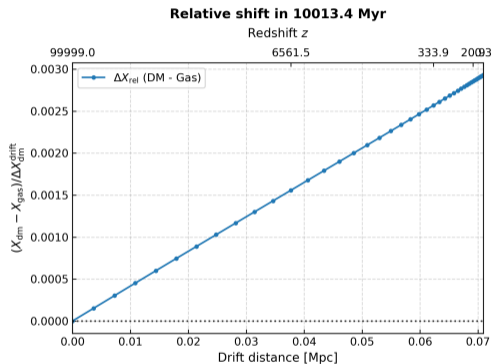
First vs final snap



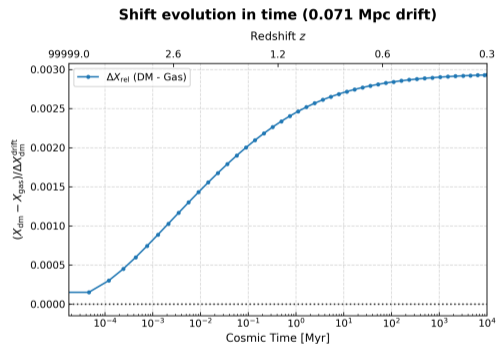
Absolute shift



Relative shift



Relative shift vs. particle **drift distance**.



Relative shift vs. **cosmic time**.

Zel'dovich test

Zel'dovich (1970)

Zel'dovich linear analytical approximation

- ▶ 1D **perturbation** on the initially uniform matter positions

$$x(q, t) = q - \frac{A}{k} \sin(kq) .$$

- ▶ **Caustic Formation**

$$\rho(x, t) = \frac{\rho_0}{1 - A(t) \cos(kq)} .$$

- ▶ **Amplitude** chosen such that

$$A = \frac{a_{\text{init}}}{a_{\text{collapse}}} .$$

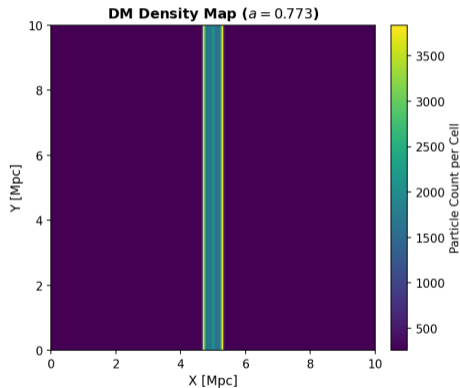
Simulation set up

- ▶ 16777216 (256^3) **DM** particles, $1.6 \cdot 10^{40}$ g each one.

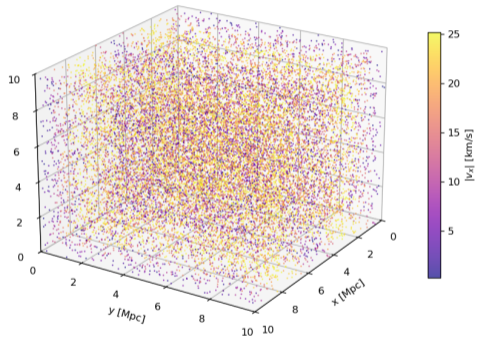
- ▶ **1D Sinusoidal** perturbation.

$$\Delta x = -\frac{1}{k} \frac{a_{\text{in}}}{a_{\text{coll}}} \sin(k \cdot x_{\text{center}}) .$$

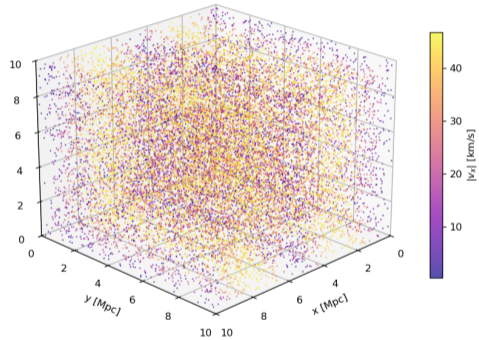
- ▶ Collapse after 13 Gyr in **EdS**, resolved with 256^3 cells (39.1 kpc resolution) in a 10 Mpc side box.



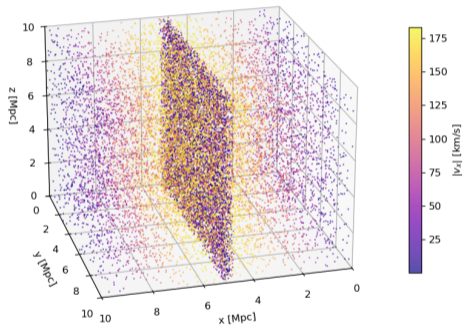
DM particles | $a = 0.013$



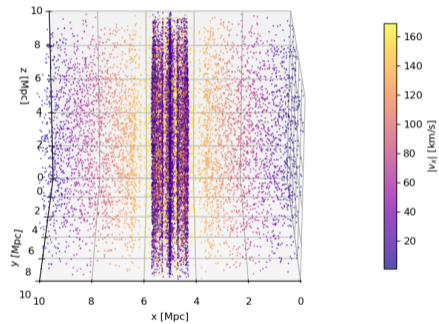
DM particles | $a = 0.044$



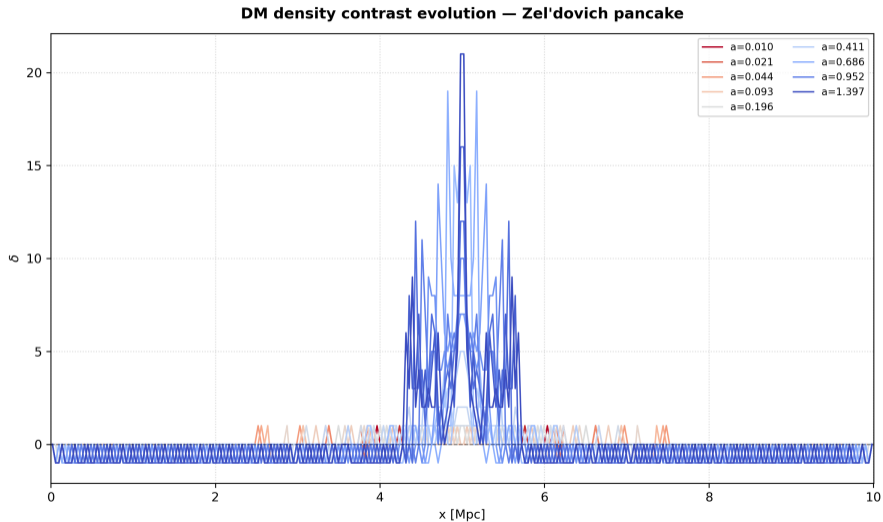
DM particles | $a = 0.686$



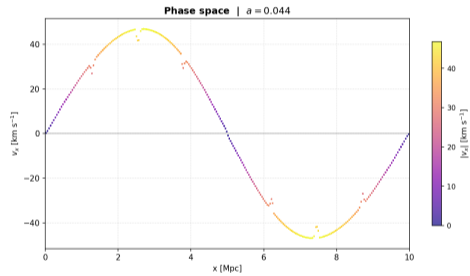
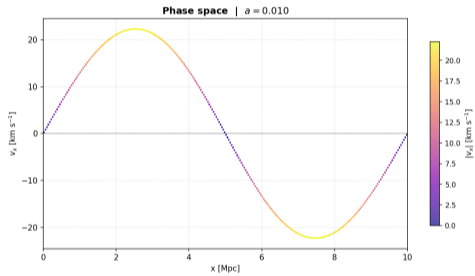
DM particles | $a = 1.397$

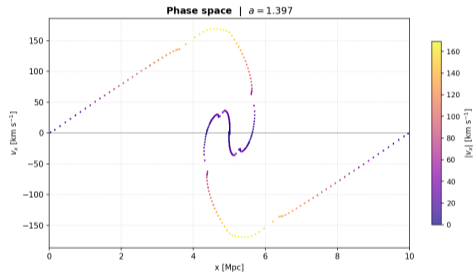
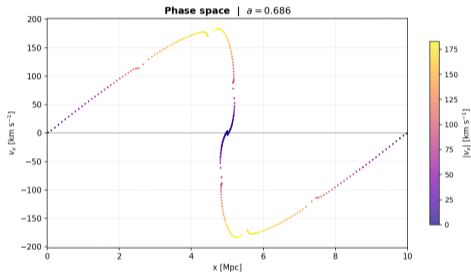


History of the collapse

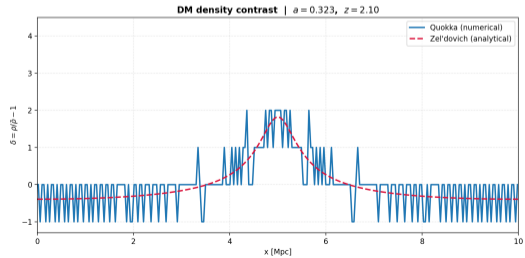
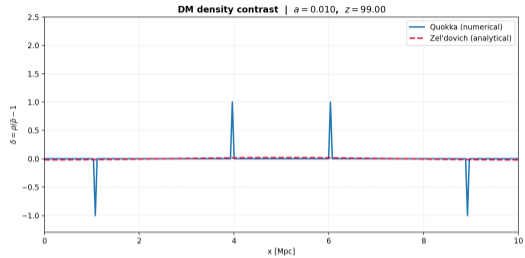


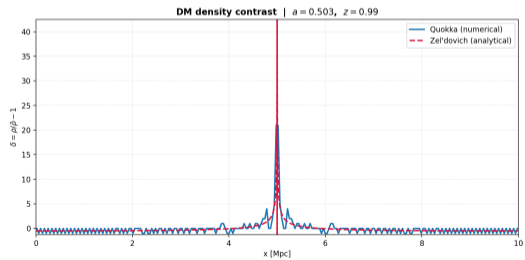
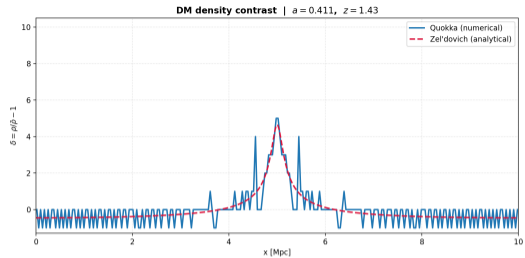
Phase space





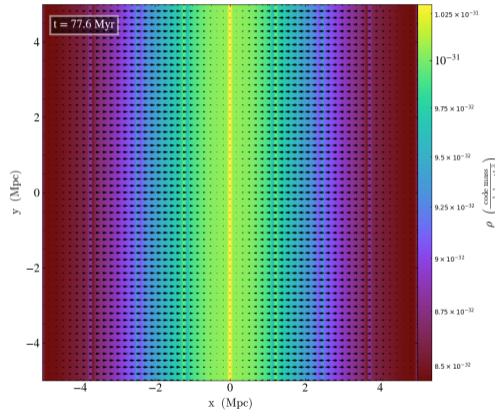
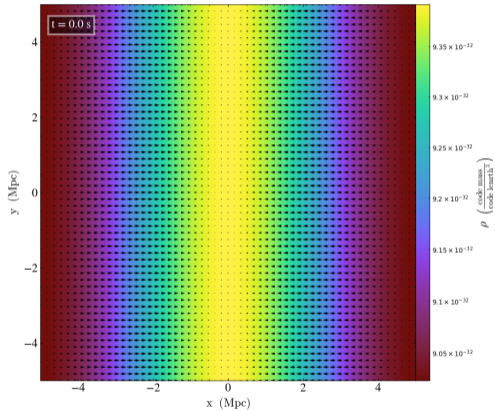
Density profiles

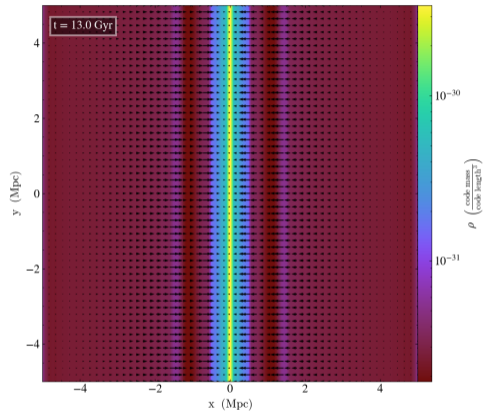
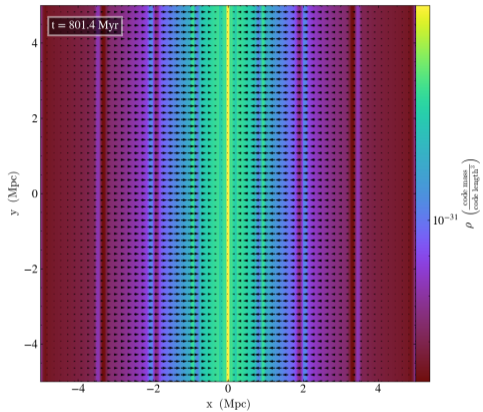




N.B. last snaps: better mass resolution!

Hydro density





Conclusion and perspectives

Conclusion and perspectives

- ▶ The implementation of a new **cosmological module for Quokka** is underway and ready for the first tests.
- ▶ **Pure expansion: Friedmann** and **hydro** solver have shown excellent agreement with analytical solutions.
- ▶ **Comoving Drift:** verified the consistency of **particle** and hydrodynamics co-evolution in an expanding background.
- ▶ **Zel'dovich Pancake:** successfully reproduced caustic formation.
- ▶ **Next steps:** new tests, AMR, radiation compatibility and simulation of a filament.



Parameters of the tests

Hydro Expansion test

Cosmological Background (EdS) and Numerical Configuration			
Hubble Parameter (h)	0.7	Grid Resolution	32^3
Matter Density (Ω_m)	1.0	Box Size (L_{com})	10^{24} cm (≈ 0.324 Mpc)
Adiabatic Index (γ)	5/3	Boundary Cond.	Periodic
Initial Epoch (a_i)	10^{-3}	Max Timesteps	2×10^8
Final Epoch (a_f)	10	CFL Coefficient	0.3
Total Time (Δt)	2.945×10^{11} yr	Solver	HLLC / PPM

Physical Quantity	Initial Value (Comoving CGS)
Density ($\rho_{com,0}$)	1.0×10^{-30} g/cm ³
Internal Energy ($e_{int,0}$)	1.5×10^{-20} erg/cm ³
Pressure (P_0)	1.0×10^{-25} erg/cm ³
Peculiar x, y, z Velocity	$5 \cdot 10^5 / \sqrt{3}$ cm/s = $5.77 \cdot 10^4$ cm/s

Cosmo Sphere test

Cosmological Background (Λ CDM) and Numerical Configuration

Hubble Parameter (h)	0.7	Grid Resolution	256^3
Matter Density (Ω_m)	0.315	Domain Width (L_{box})	0.50 Mpc
Radiation Density (Ω_r)	9.2618×10^{-5}	Single Cell Size (Δx)	1.95 kpc
Dark Energy (Ω_Λ)	0.685	Initial Drift (v_x)	1000 km/s
Distance covered	70.9 kpc	Total time	10 Gyr ($a_{\text{in}} = 10^{-5}$)

-> DM (X,Y,Z): (0.3209, 0.2500, 0.2500) Mpc

-> Gas (X,Y,Z): (0.3207, 0.2500, 0.2500) Mpc

Total distance traveled by DM : 70.9 kpc

Final shift (DM - Gas) : 0.21 kpc (0.11 cells)

Final DM velocity: $1.29 \cdot 10^3$ cm/s

Zel'dovich parameters

Cosmological Background (EdS) and Numerical Configuration

Hubble Parameter (h)	0.7	Adiabatic Index (γ)	5/3
Matter Density (Ω_m)	1	Domain Width (L_{box})	10 Mpc
DM Density (Ω_{dm})	0.99	Grid Resolution	256^3
Ordinary Matter Dens. (Ω_b)	0.01	Single Cell Size (Δx)	39.1 kpc
Initial Scale Factor (a_{in})	0.01	Total Time	13 Gyr
Collapse Scale Factor (a_{coll})	0.5	DM particles	16777216
Final Scale Factor (a_{fin})	1.25	Mass per Particle	$1.6 \cdot 10^{40}$ g

Only gas Zel'dovich pancake

Only gas Zel'dovich

