PARTICLE DIFFUSION AND ACCELERATION MODELING WITH STOCHASTIC DIFFERENTIAL EQUATIONS

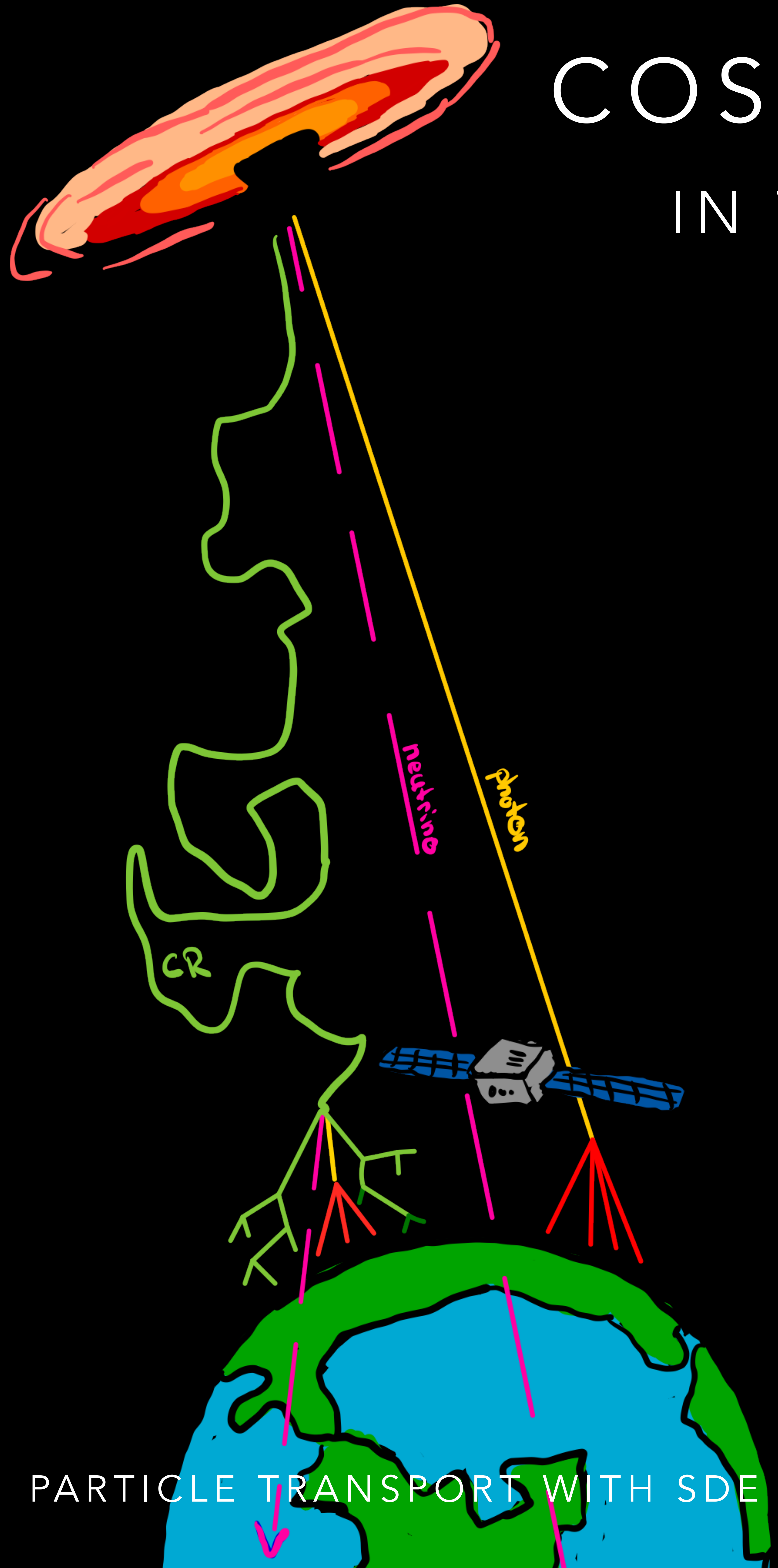
ASTROPARTICLE SYMPOSIUM 2025 - 18.11.2025

SOPHIE AERDKER, APC PARIS & RUB

WITH LUKAS MERTEN, FREDERIC EFFENBERGER, HORST FICHTNER, JULIA TJUS, ROARK HABEGGER, ELLEN ZWEIBEL, MARTIN LEMOINE

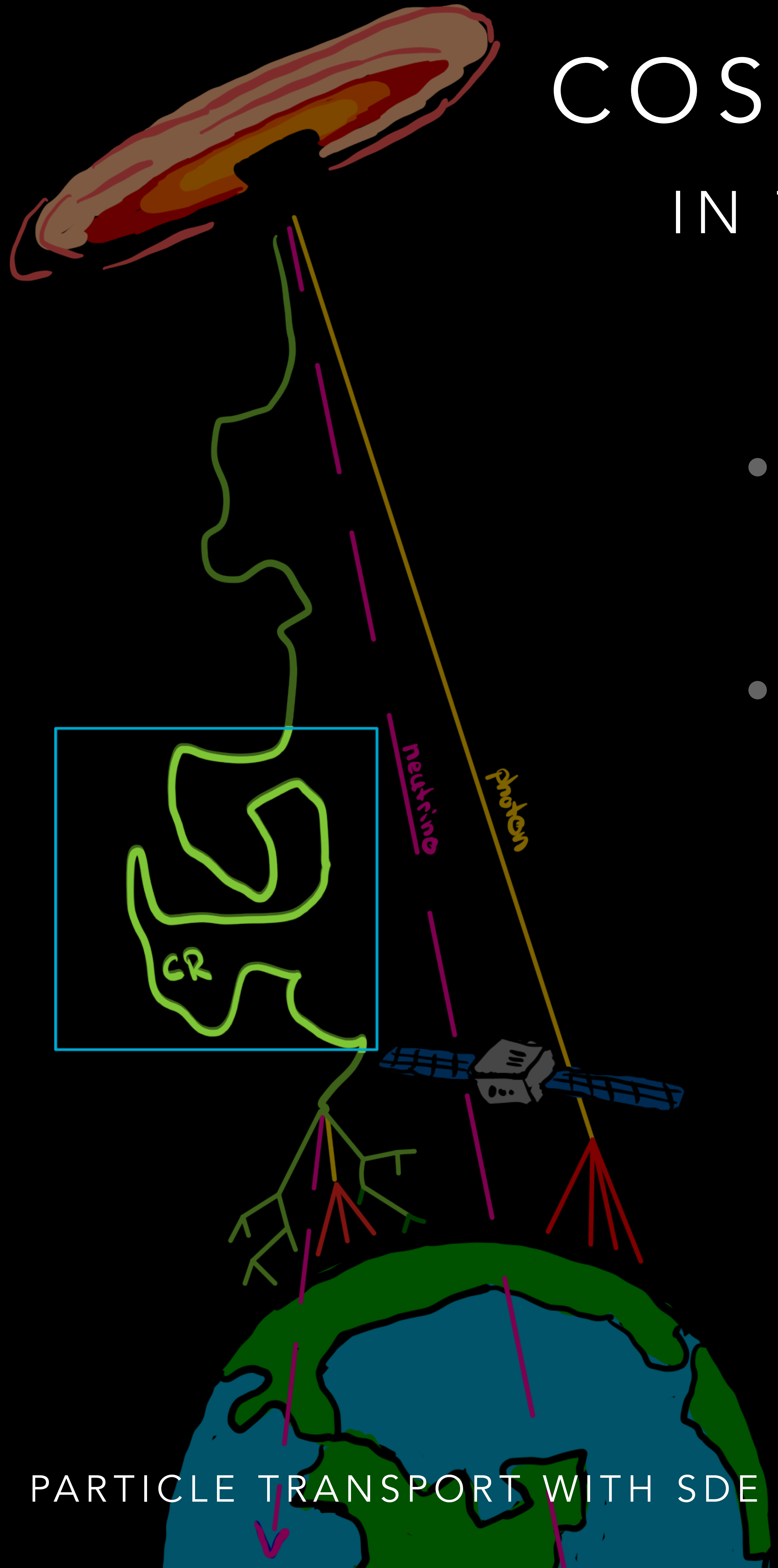
COSMIC RAY TRANSPORT

IN TURBULENT MAGNETIC FIELDS

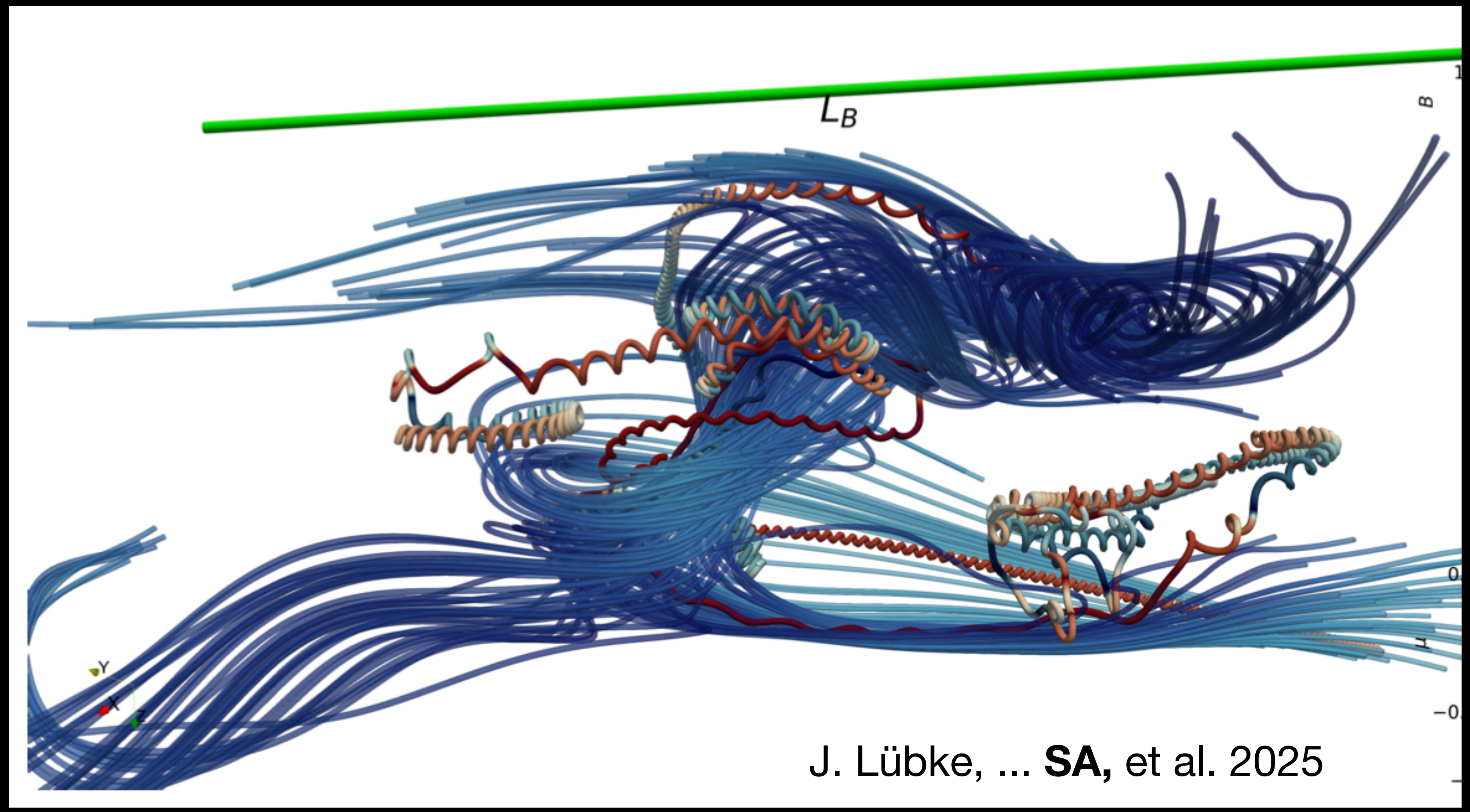


COSMIC RAY TRANSPORT

IN TURBULENT MAGNETIC FIELDS



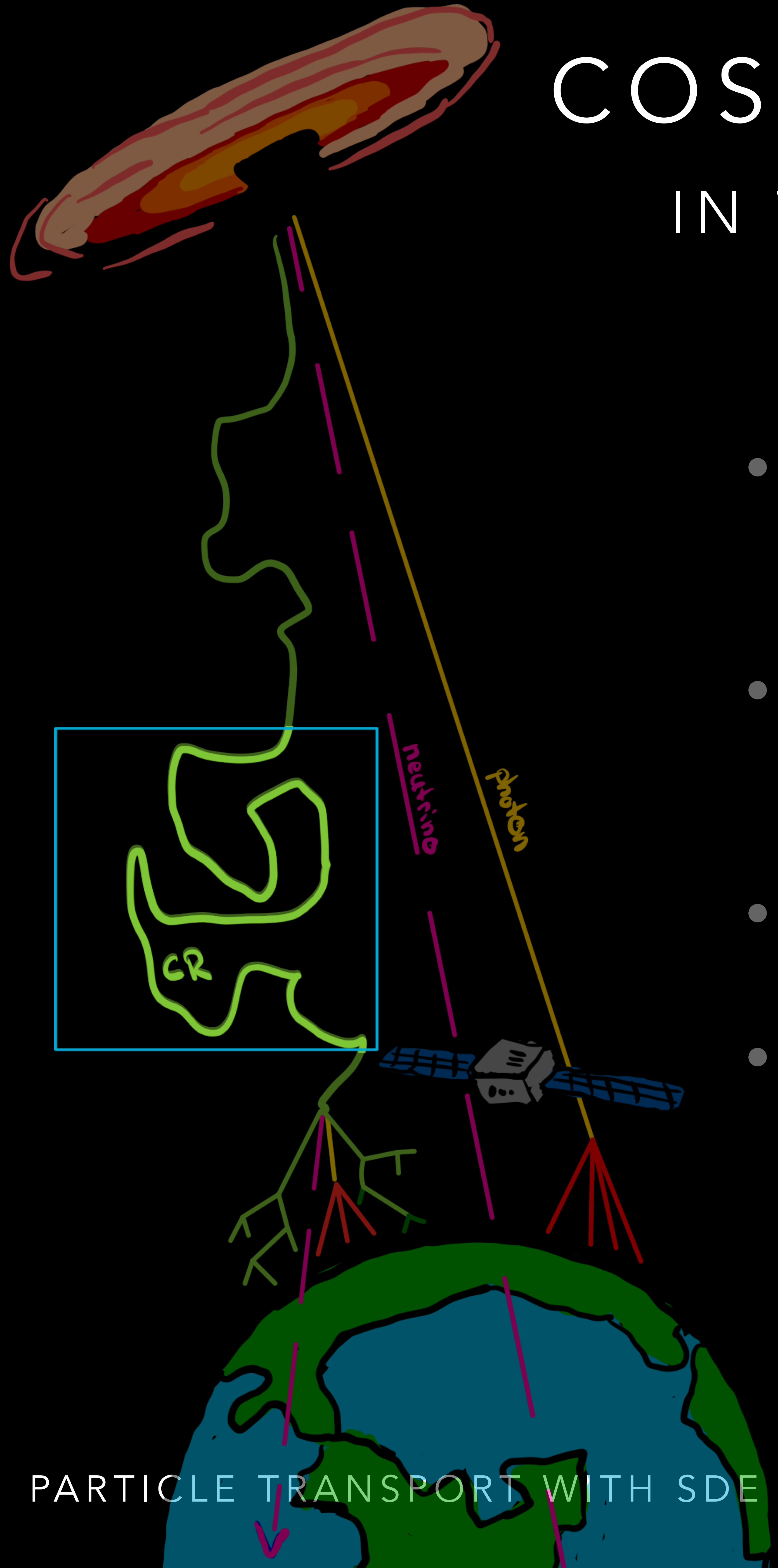
- Charged particles follow magnetic field lines & scatter on inhomogeneties
- Good knowledge of the magnetic field & turbulence



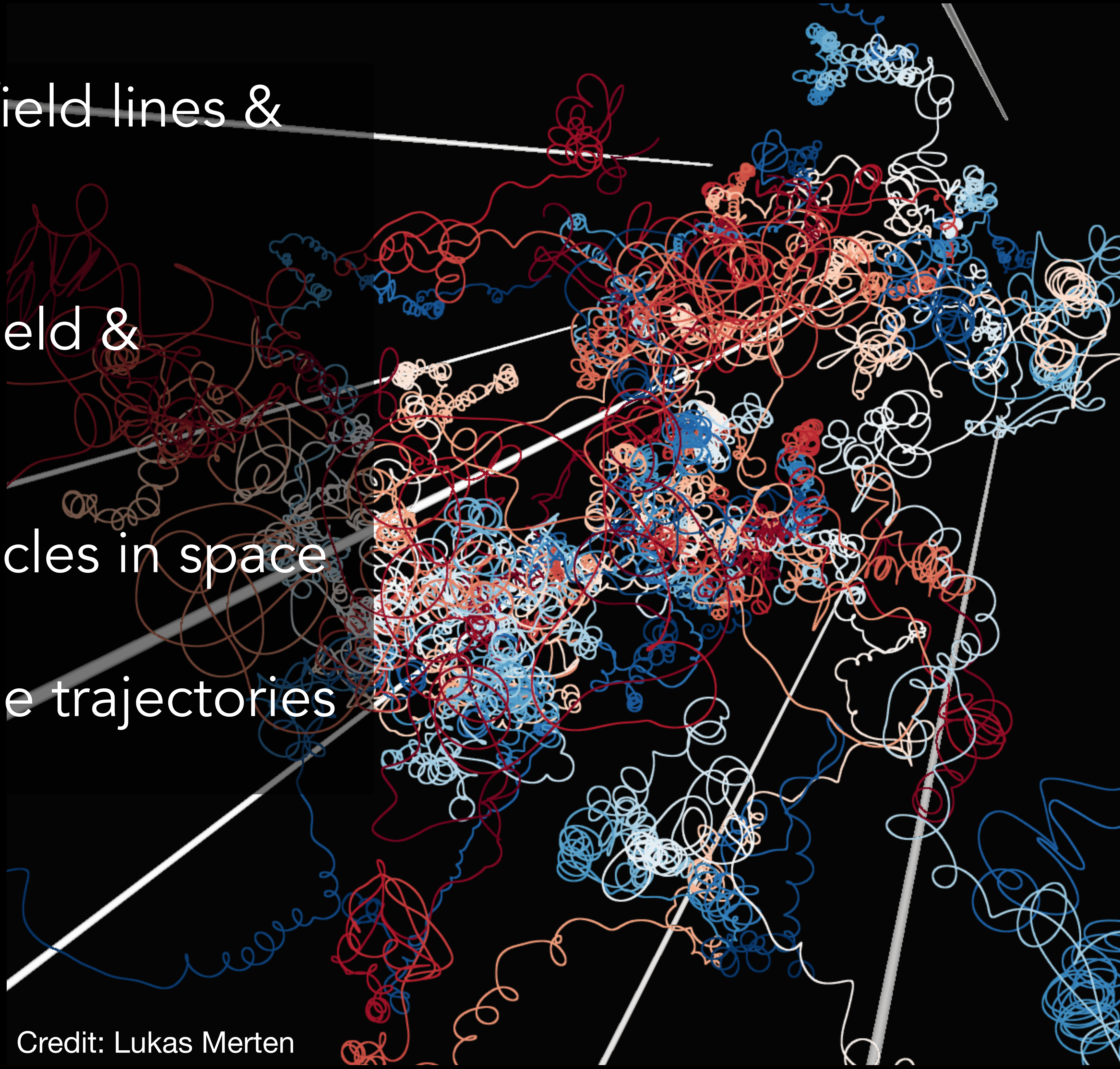
J. Lübke, ... **SA,** et al. 2025

COSMIC RAY TRANSPORT

IN TURBULENT MAGNETIC FIELDS



- Charged particles follow magnetic field lines & scatter on inhomogeneties
- Good knowledge of the magnetic field & turbulence
- Scattering leads to diffusion of particles in space
- Unfeasible to track individual particle trajectories


Credit: Lukas Merten

ENSEMBLE AVERAGED APPROACH

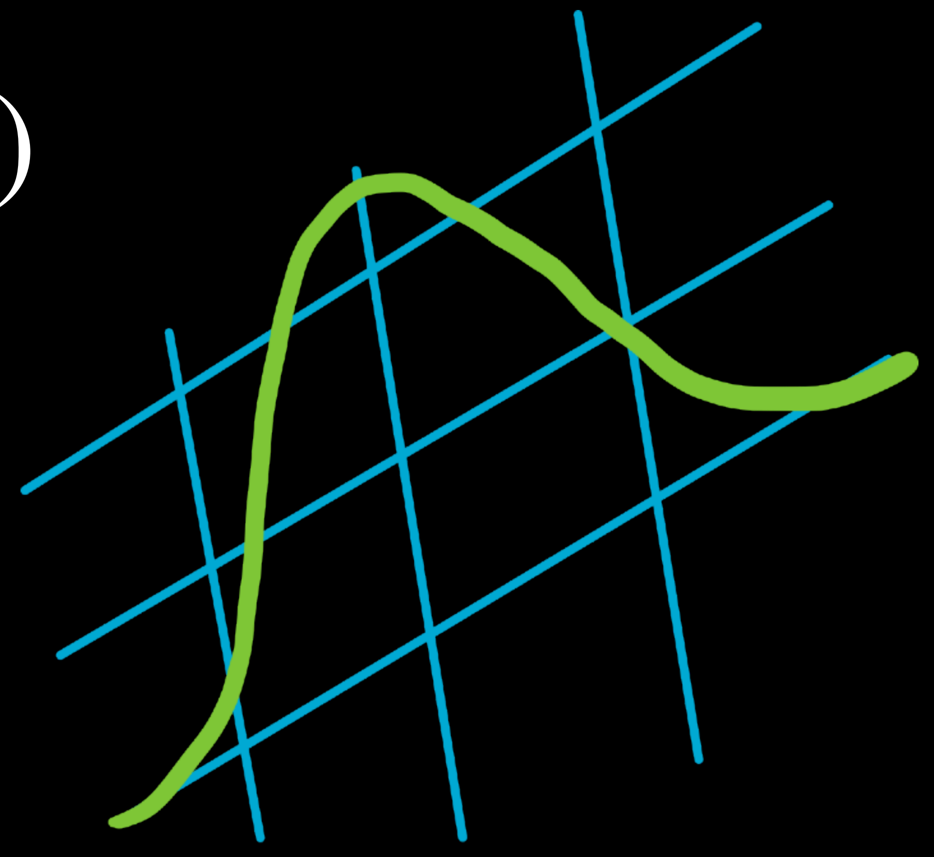
TRANSPORT EQUATION

$$\frac{\partial f}{\partial t} + \underbrace{\vec{u} \cdot \nabla f}_{\text{advection}} = \underbrace{\nabla \cdot \left(\hat{\kappa} \nabla f\right)}_{\text{spatial diffusion}} + \underbrace{\frac{1}{p^2} \frac{\partial}{\partial p} \left(p^2 D \frac{\partial f}{\partial p} \right)}_{\text{momentum diffusion}} + \underbrace{\frac{p}{3} \left(\nabla \cdot \vec{u} \right) \frac{\partial f}{\partial p}}_{\text{adiabatic energy change}} + S(\vec{x}, p, t)$$

ENSEMBLE AVERAGED APPROACH

TRANSPORT EQUATION

$$\frac{\partial f}{\partial t} + \underbrace{\vec{u} \cdot \nabla f}_{\text{advection}} = \underbrace{\nabla \cdot \left(\hat{\kappa} \nabla f\right)}_{\text{spatial diffusion}} + \underbrace{\frac{1}{p^2}\frac{\partial}{\partial p}\left(p^2 D \frac{\partial f}{\partial p}\right)}_{\text{momentum diffusion}} + \underbrace{\frac{p}{3}\left(\nabla \cdot \vec{u}\right)\frac{\partial f}{\partial p}}_{\text{adiabatic energy change}} + S(\vec{x}, p, t)$$



ENSEMBLE AVERAGED APPROACH

TRANSPORT EQUATION - FOKKER-PLANCK EQUATION

$$\frac{\partial n}{\partial t} = \frac{1}{2}\nabla^2(2\hat{\kappa} n) - \nabla\left[\left(\nabla\hat{\kappa} + \vec{u}\right) n\right] + \frac{1}{2}\frac{\partial^2}{\partial p^2}(2Dn) - \frac{\partial}{\partial p}\left[\left(\frac{\partial D}{\partial p} + \frac{2D}{p} - \frac{p}{3}\nabla \cdot \vec{u}\right) n\right] + S_n$$

ENSEMBLE AVERAGED APPROACH

TRANSPORT EQUATION & STOCHASTIC DIFFERENTIAL EQUATIONS

$$\frac{\partial n}{\partial t} = \frac{1}{2}\nabla^2(2\hat{\kappa}n) - \nabla\left[\left(\nabla\hat{\kappa} + \vec{u}\right)n\right] + \frac{1}{2}\frac{\partial^2}{\partial p^2}(2Dn) - \frac{\partial}{\partial p}\left[\left(\frac{\partial D}{\partial p} + \frac{2D}{p} - \frac{p}{3}\nabla\cdot\vec{u}\right)n\right] + S_n$$

FROM FOKKER-PLANCK TO STOCHASTIC DIFFERENTIAL EQUATIONS:

$$\mathrm{d}\vec{x} = \left(\nabla\cdot\hat{\kappa} + \vec{u}\right)\mathrm{d}t + \sqrt{2\hat{\kappa}}\,\mathrm{d}\vec{\omega}_{x,t} \qquad \mathrm{d}p = \left(\frac{2D}{p} + \frac{\partial D}{\partial p} - \frac{p}{3}\nabla\cdot\vec{u}\right)\mathrm{d}t + \sqrt{2D}\,\mathrm{d}\omega_{p,t}$$

ENSEMBLE AVERAGED APPROACH

TRANSPORT EQUATION & STOCHASTIC DIFFERENTIAL EQUATIONS

$$\frac{\partial n}{\partial t} = \frac{1}{2}\nabla^2(2\hat{\kappa}n) - \nabla\left[\left(\nabla\hat{\kappa} + \vec{u}\right)n\right] + \frac{1}{2}\frac{\partial^2}{\partial p^2}(2Dn) - \frac{\partial}{\partial p}\left[\left(\frac{\partial D}{\partial p} + \frac{2D}{p} - \frac{p}{3}\nabla\cdot\vec{u}\right)n\right] + S_n$$

FROM FOKKER-PLANCK TO STOCHASTIC DIFFERENTIAL EQUATIONS:

$$\mathrm{d}\vec{x} = \left(\nabla\cdot\hat{\kappa} + \vec{u}\right)\mathrm{d}t + \sqrt{2\hat{\kappa}}\,\mathrm{d}\vec{\omega}_{x,t} \qquad \mathrm{d}p = \left(\frac{2D}{p} + \frac{\partial D}{\partial p} - \frac{p}{3}\nabla\cdot\vec{u}\right)\mathrm{d}t + \sqrt{2D}\,\mathrm{d}\omega_{p,t}$$

Pseudo-particles are propagated with Stochastic Differential Equations

CR/Propa
Cosmic Ray Propagation Framework

L. Merten & SA, CPC, 2025

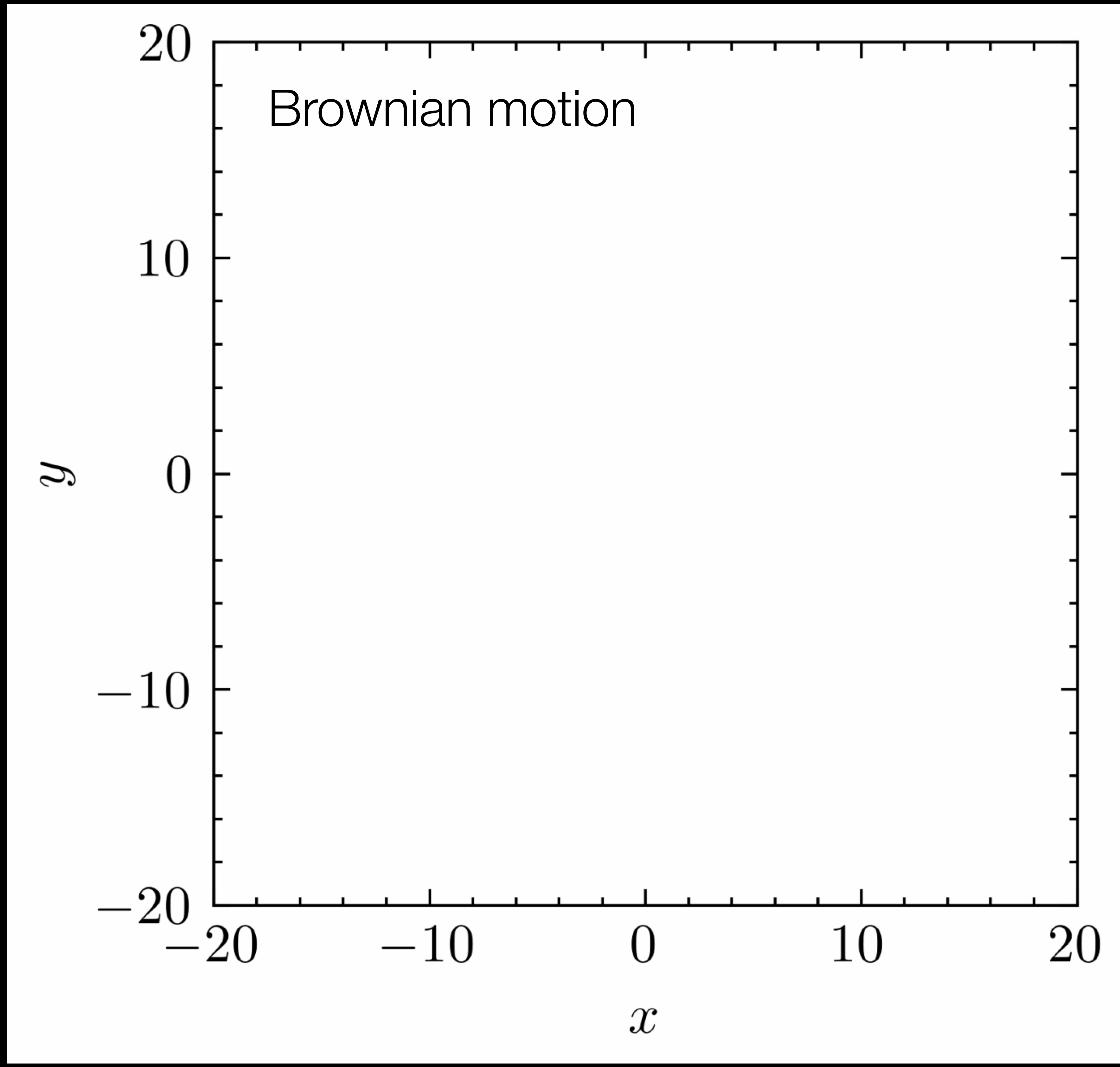
BROWNIAN MOTION

INTEGRATING STOCHASTIC DIFFERENTIAL EQUATIONS

- Pure diffusion, integrated with **Euler-Maruyama** scheme:

$$\vec{x}_{t+1} = \vec{x}_t + \sqrt{2\hat{\kappa}}\sqrt{\Delta t}\vec{\eta}_{x,t}$$

- Random numbers η drawn from a **Gaussian distribution**



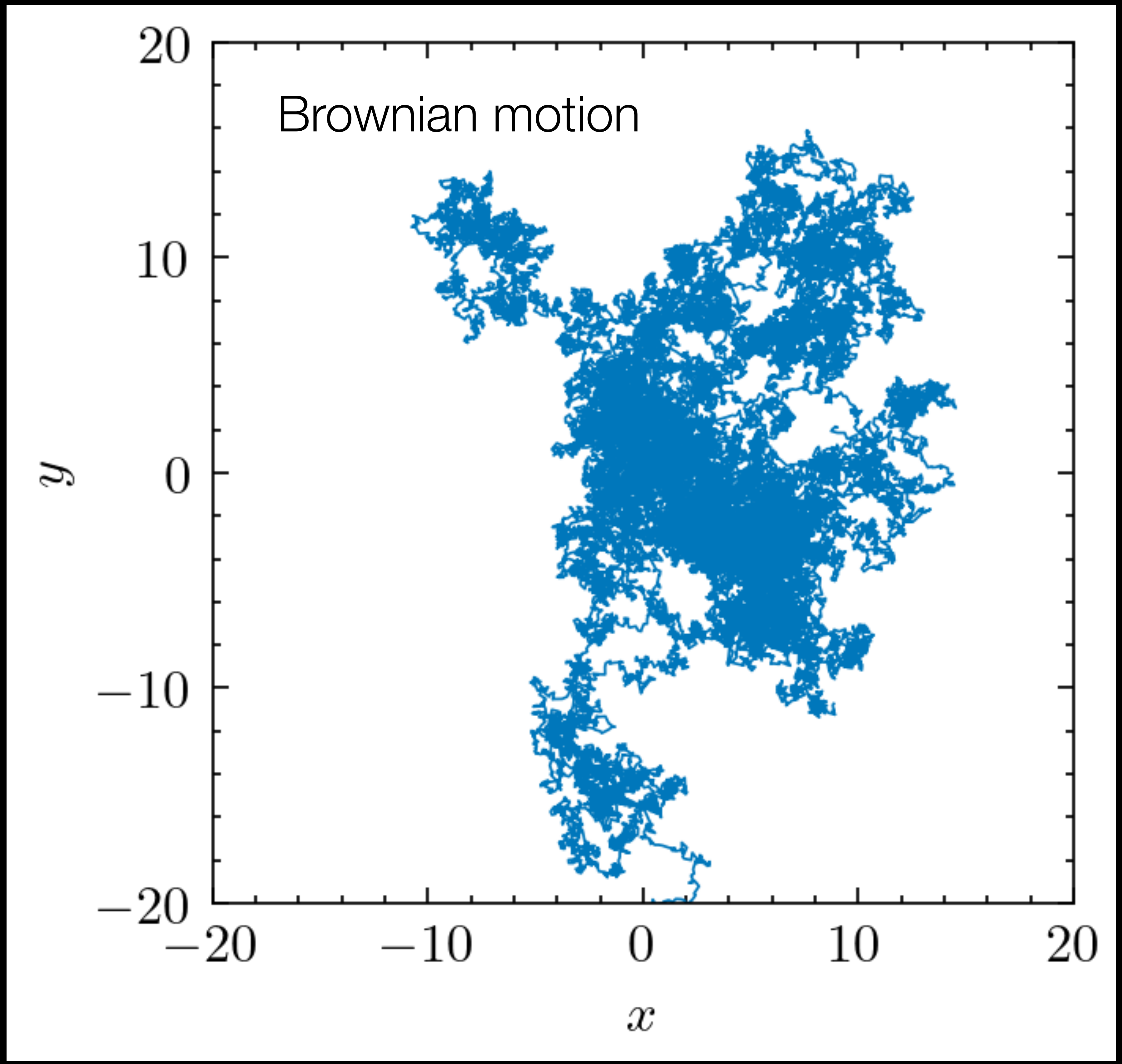
BROWNIAN MOTION

INTEGRATING STOCHASTIC DIFFERENTIAL EQUATIONS

- Pure diffusion, integrated with **Euler-Maruyama** scheme:

$$\vec{x}_{t+1} = \vec{x}_t + \sqrt{2\hat{\kappa}}\sqrt{\Delta t}\vec{\eta}_{x,t}$$

- Random numbers η drawn from a **Gaussian distribution**



BROWNIAN MOTION

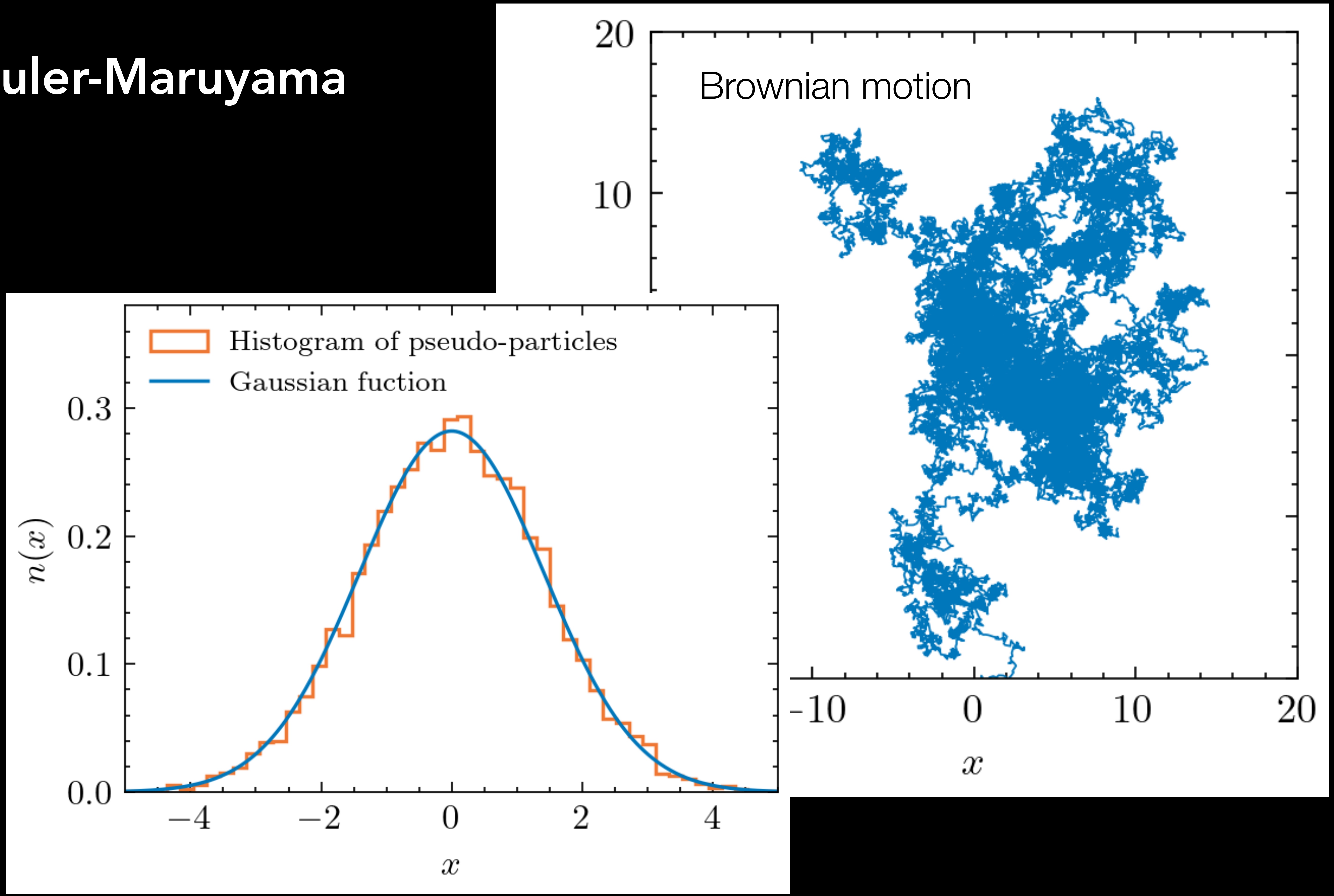
INTEGRATING STOCHASTIC DIFFERENTIAL EQUATIONS

- Pure diffusion, integrated with **Euler-Maruyama** scheme:

$$\vec{x}_{t+1} = \vec{x}_t + \sqrt{2\hat{\kappa}}\sqrt{\Delta t}\vec{\eta}_{x,t}$$

- Random numbers η drawn from a **Gaussian distribution**

- Recover macroscopic quantities



PARTICLE SCATTERING

FROM PITCH-ANGLE TO SPATIAL DIFFUSION

- Properties of the turbulent magnetic field encoded into diffusion coefficient $\hat{\kappa}$ and stochastic driver $\mathrm{d}W_t$
- Scattering in pitch-angle leads to diffusion along the magnetic field

$$d\mu = -2\mu D_0 \mathrm{d}t + \sqrt{2D_0(1-\mu^2)}\mathrm{d}W_\mu$$

$$ds = v\mu \mathrm{d}t$$

PARTICLE SCATTERING

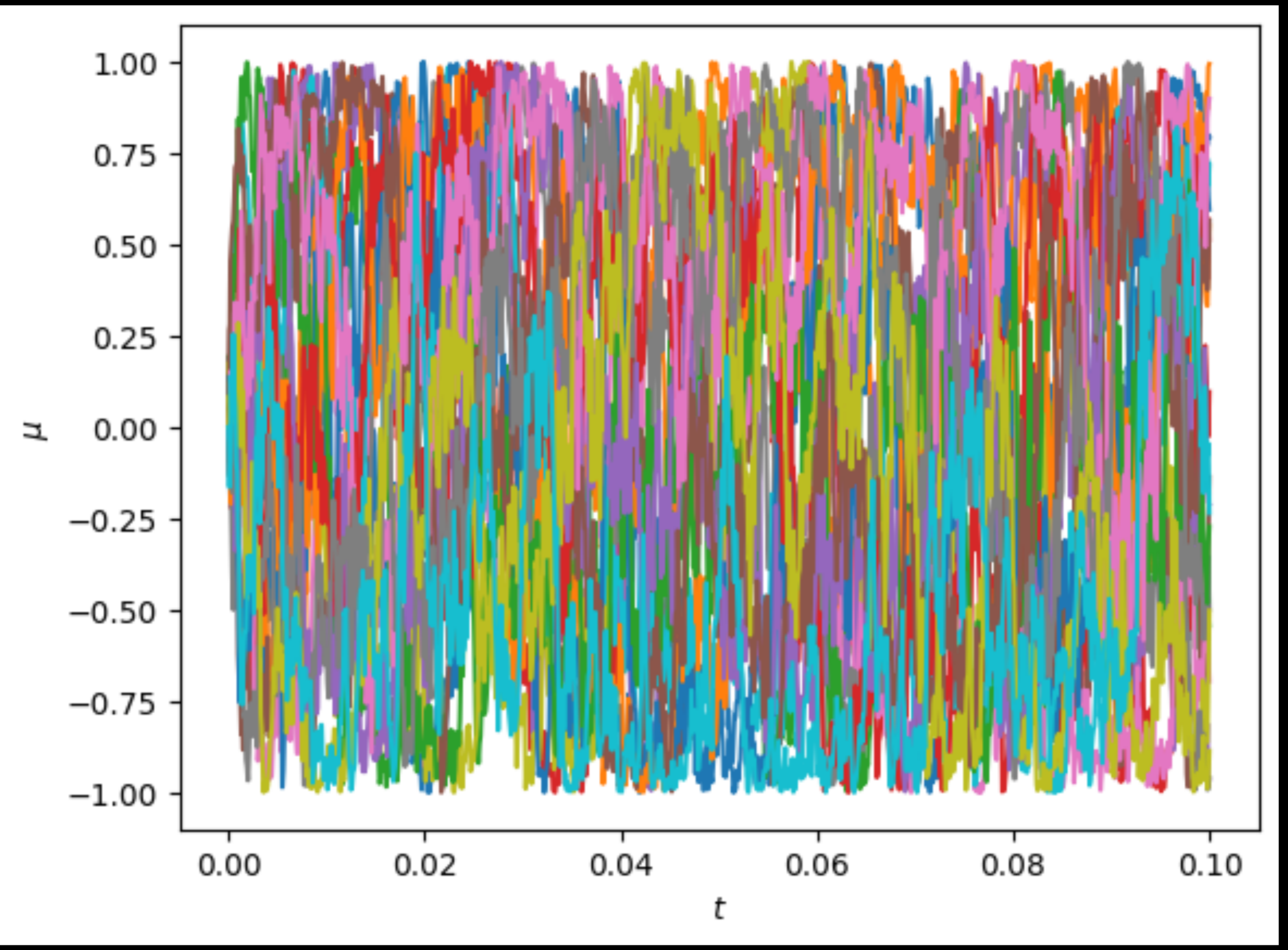
FROM PITCH-ANGLE TO SPATIAL DIFFUSION

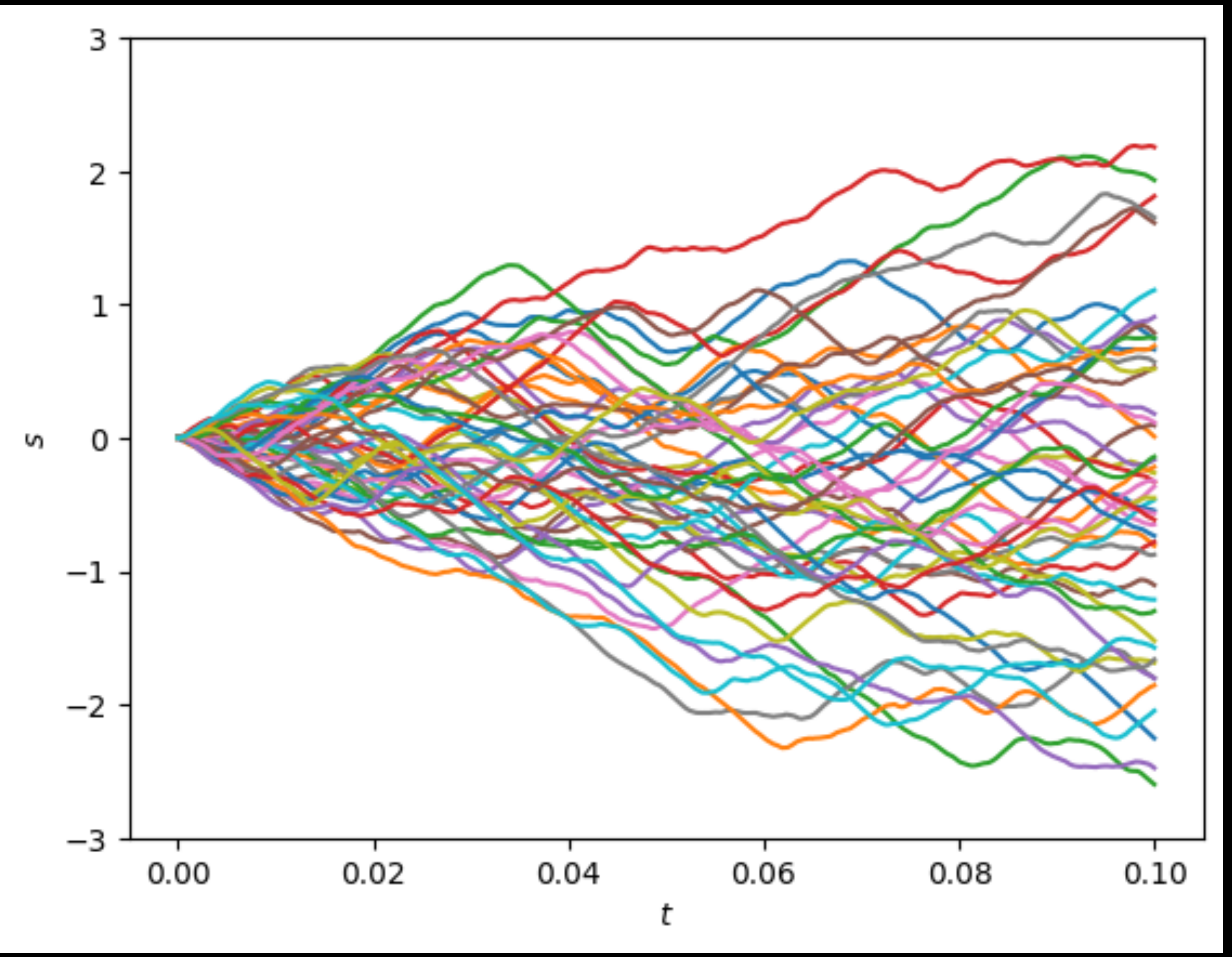
- Properties of the turbulent magnetic field encoded into diffusion coefficient $\hat{\kappa}$ and stochastic driver $\mathrm{d}W_t$

- Scattering in pitch-angle leads to diffusion along the magnetic field

$$d\mu = -2\mu D_0 \mathrm{d}t + \sqrt{2D_0(1-\mu^2)}\mathrm{d}W_\mu$$

$$ds = v\mu \mathrm{d}t$$

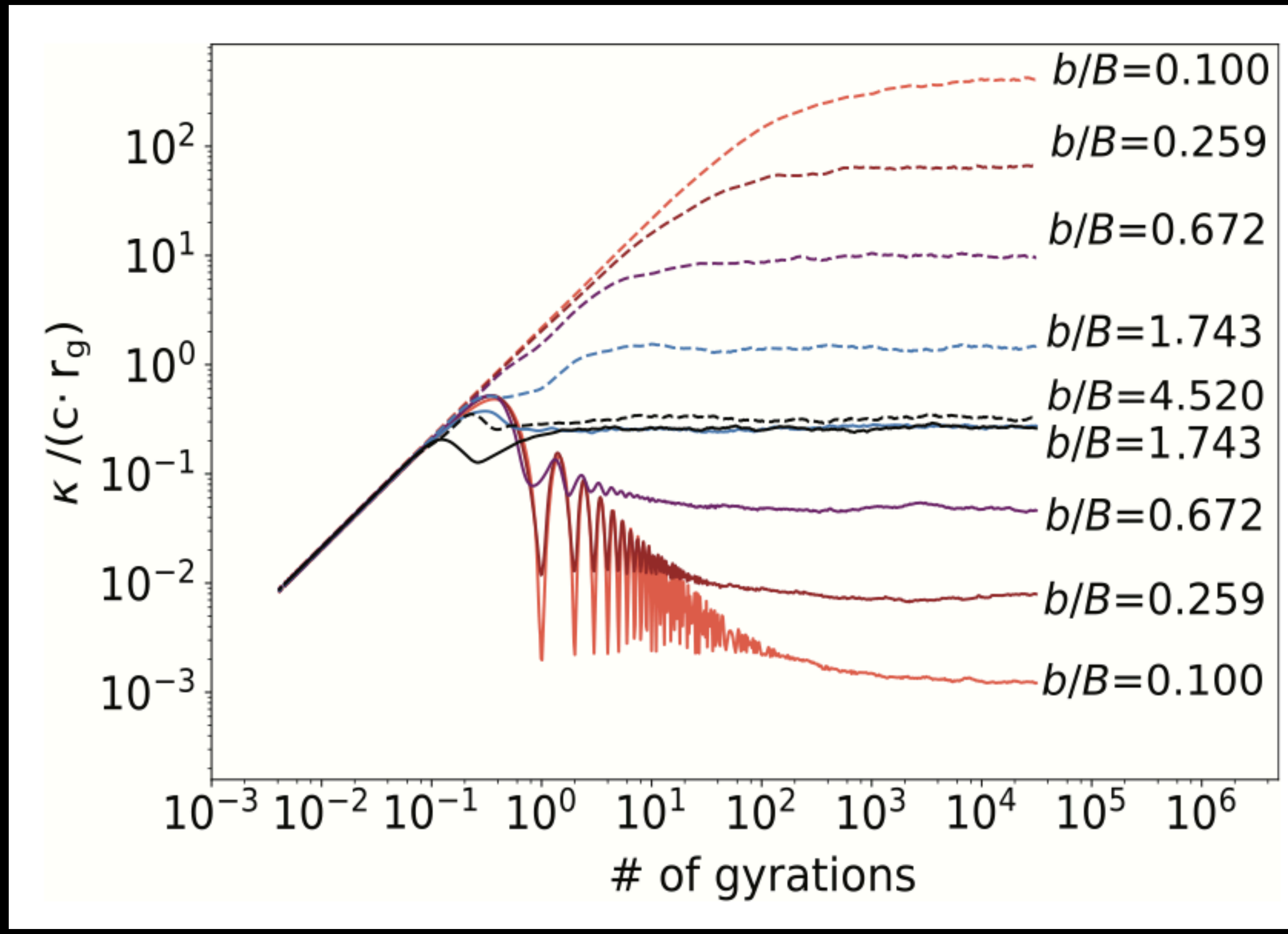




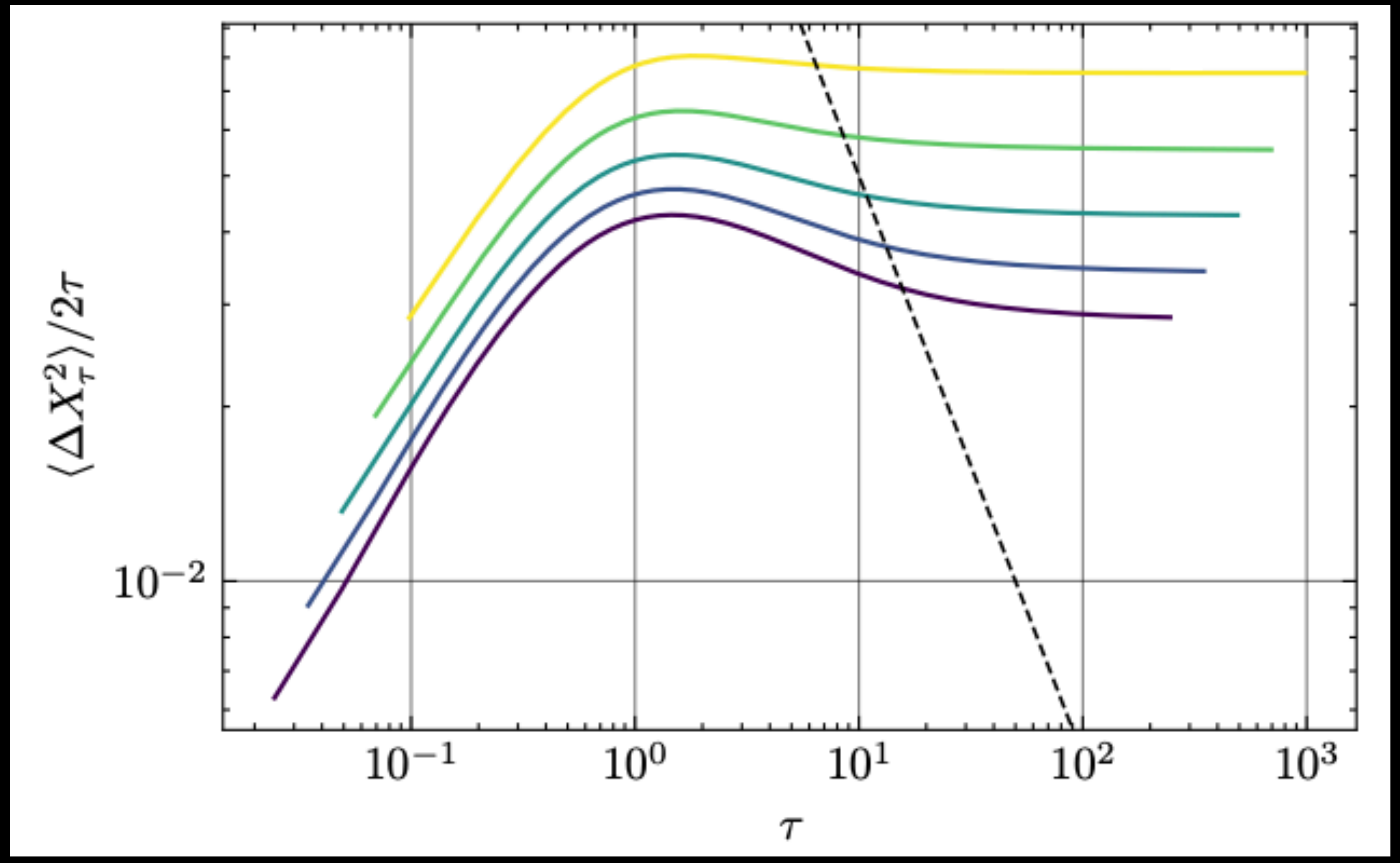
PARTICLE SCATTERING

FROM PITCH-ANGLE TO SPATIAL DIFFUSION

- Properties of the turbulent magnetic field encoded into diffusion coefficient $\hat{\kappa}$ and stochastic driver $\mathrm{d}W_t$
- Scattering in pitch-angle leads to diffusion along the magnetic field
- Running diffusion coefficient: $< (\Delta x)^2 > /2t$



Particle transport in synthetic turbulence: Reichherzer, et al. 2020



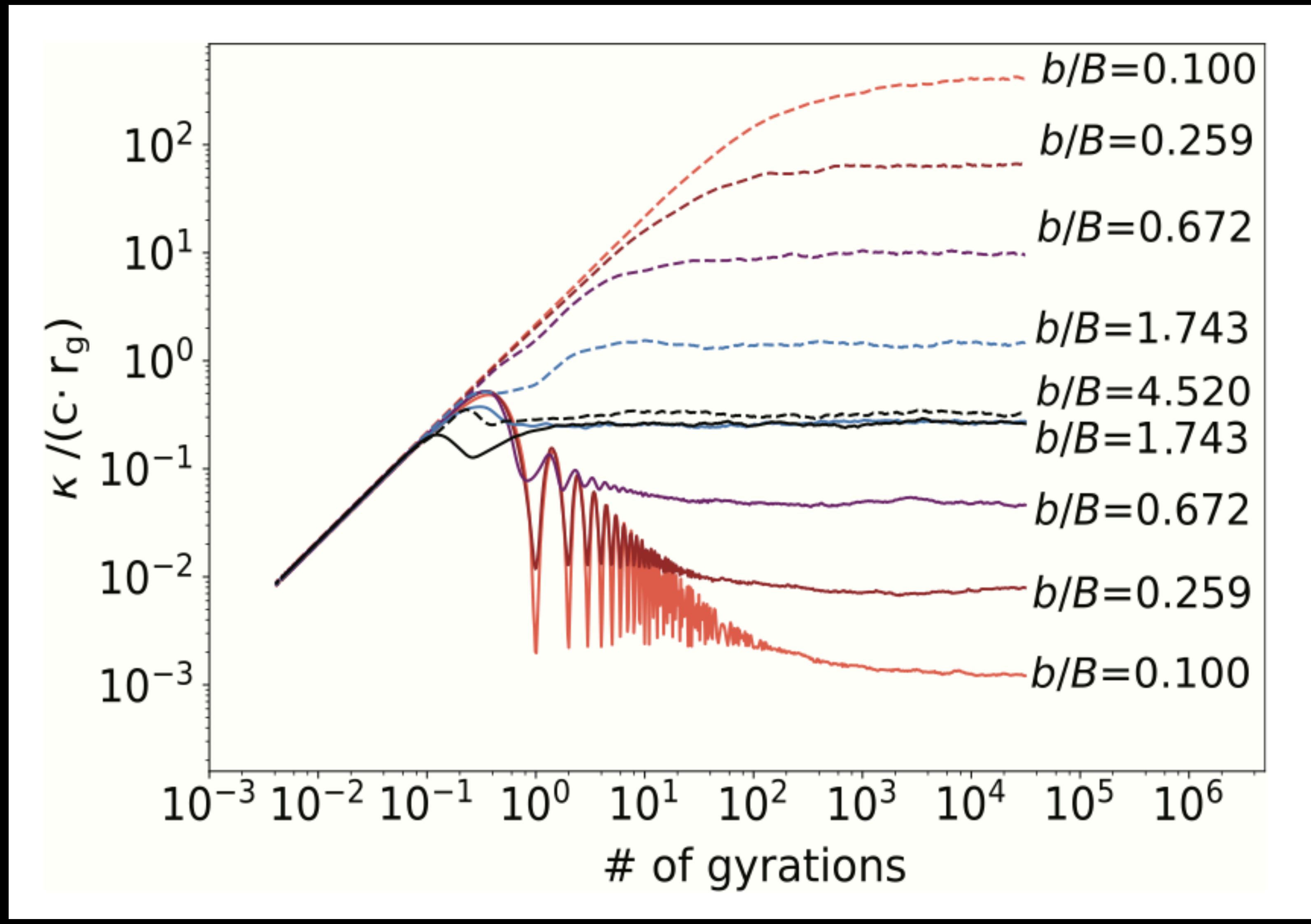
Particle transport in MHD turbulence: Lübke, ... SA, et al. 2025

PARTICLE SCATTERING

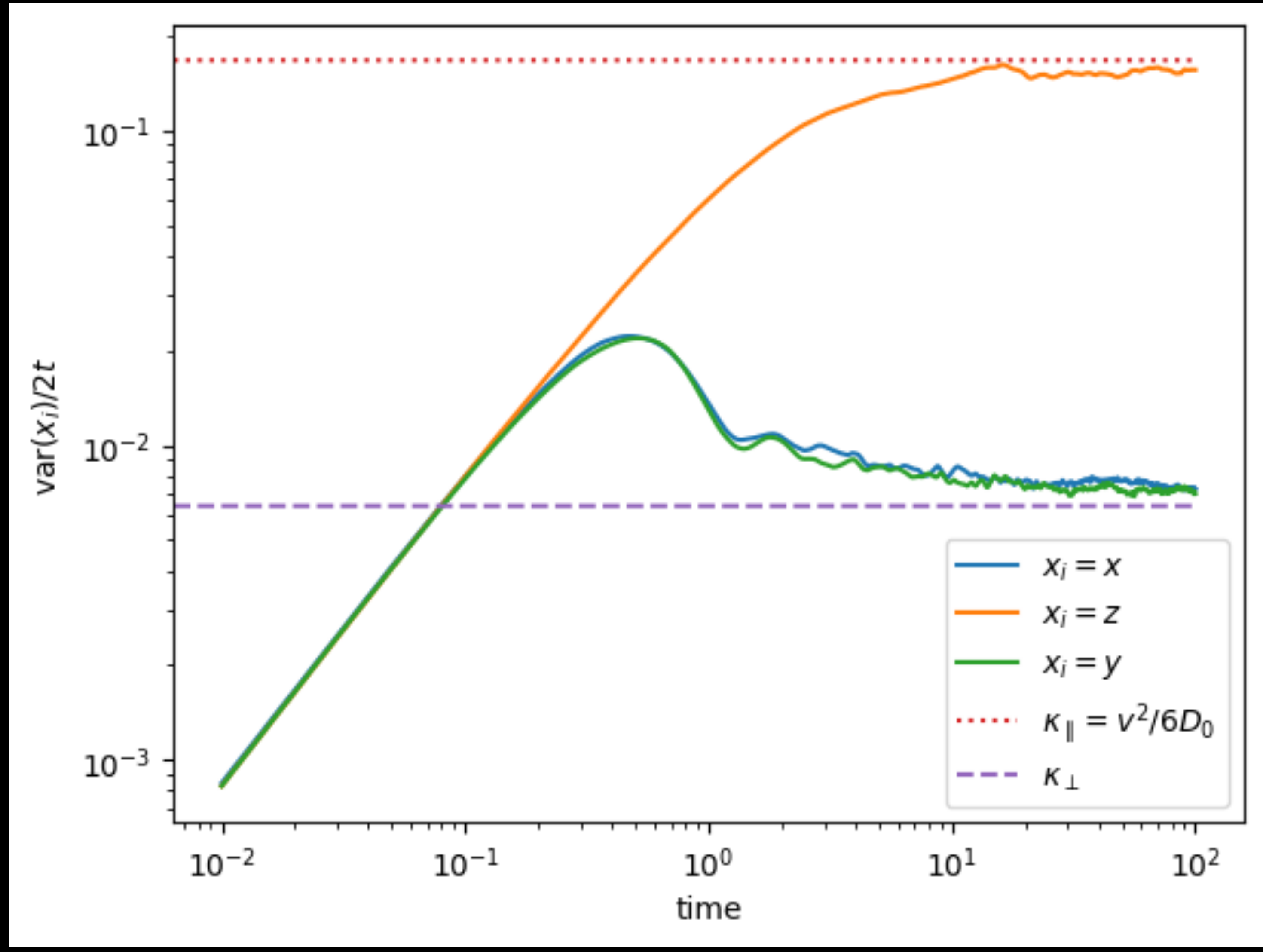
FROM PITCH-ANGLE TO SPATIAL DIFFUSION

- Properties of the turbulent magnetic field encoded into diffusion coefficient $\hat{\kappa}$ and stochastic driver $\mathrm{d}W_t$
- Scattering in pitch-angle leads to diffusion along the magnetic field
- Running diffusion coefficient: $<(\Delta x)^2>/2t$

$$\kappa_{\parallel} = \frac{v^2 \tau_{\parallel}}{3}$$



Particle transport in synthetic turbulence: Reichherzer, et al. 2020



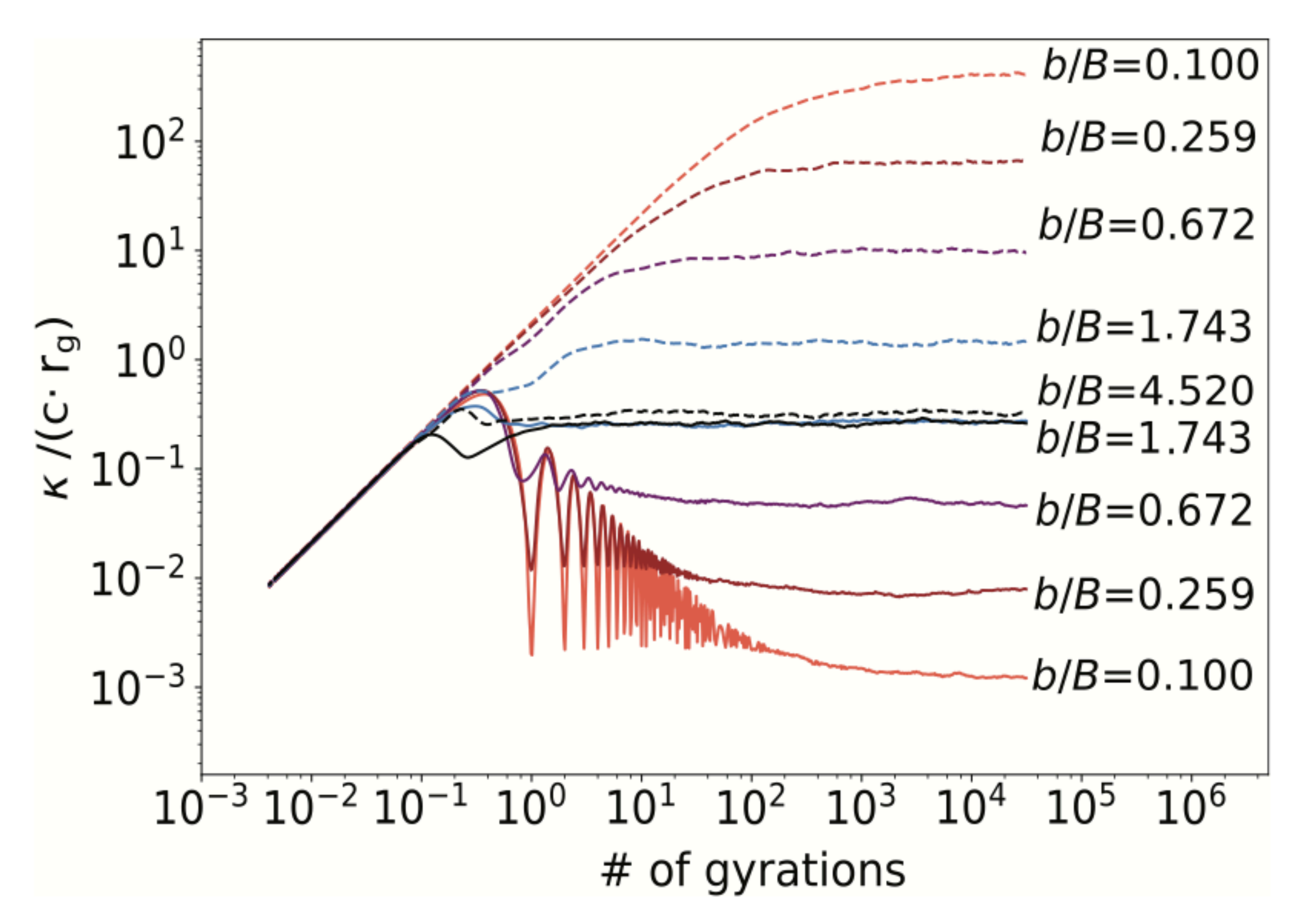
PARTICLE SCATTERING

FROM PITCH-ANGLE TO SPATIAL DIFFUSION

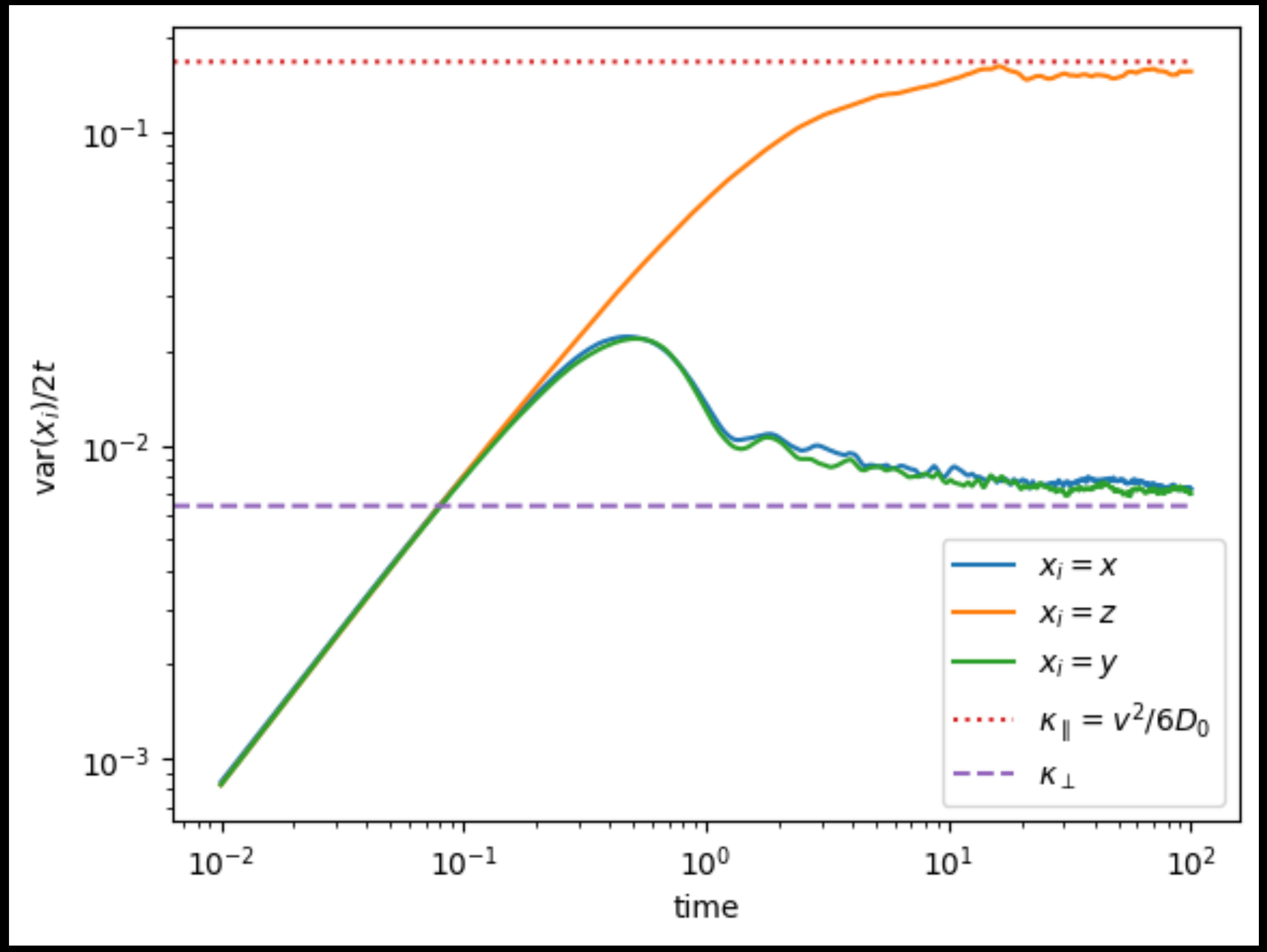
- Properties of the turbulent magnetic field encoded into diffusion coefficient $\hat{\kappa}$ and stochastic driver $\mathrm{d}W_t$
- Scattering in pitch-angle leads to diffusion along the magnetic field
- Running diffusion coefficient: $<(\Delta x)^2>/2t$

$$\kappa_{\parallel} = \frac{v^2 \tau_{\parallel}}{3}$$

CRPropa



Particle transport in synthetic turbulence: Reichherzer, et al. 2020



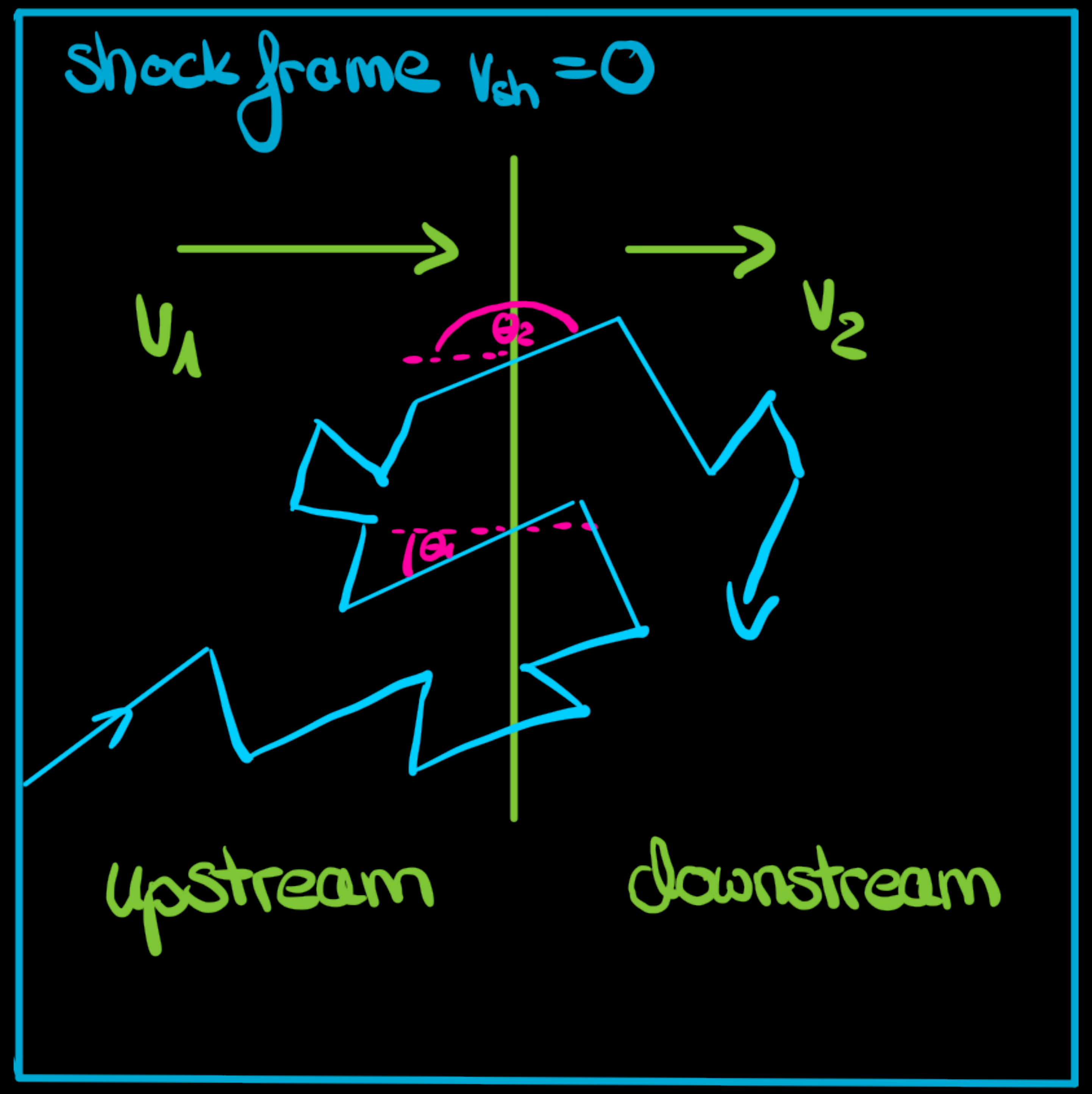
ACCELERATION MODELS

PARTICLE ACCELERATION

DIFFUSIVE SHOCK ACCELERATION

$$\mathrm{d}\vec{x} = \left(\nabla \cdot \hat{\kappa} + \vec{u}(x) \right) \mathrm{d}t + \sqrt{2\hat{\kappa}}\, \mathrm{d}\vec{\omega}_{x,t}$$

$$\mathrm{d}p = -\frac{p}{3} \nabla \cdot \vec{u}\, \mathrm{d}t$$

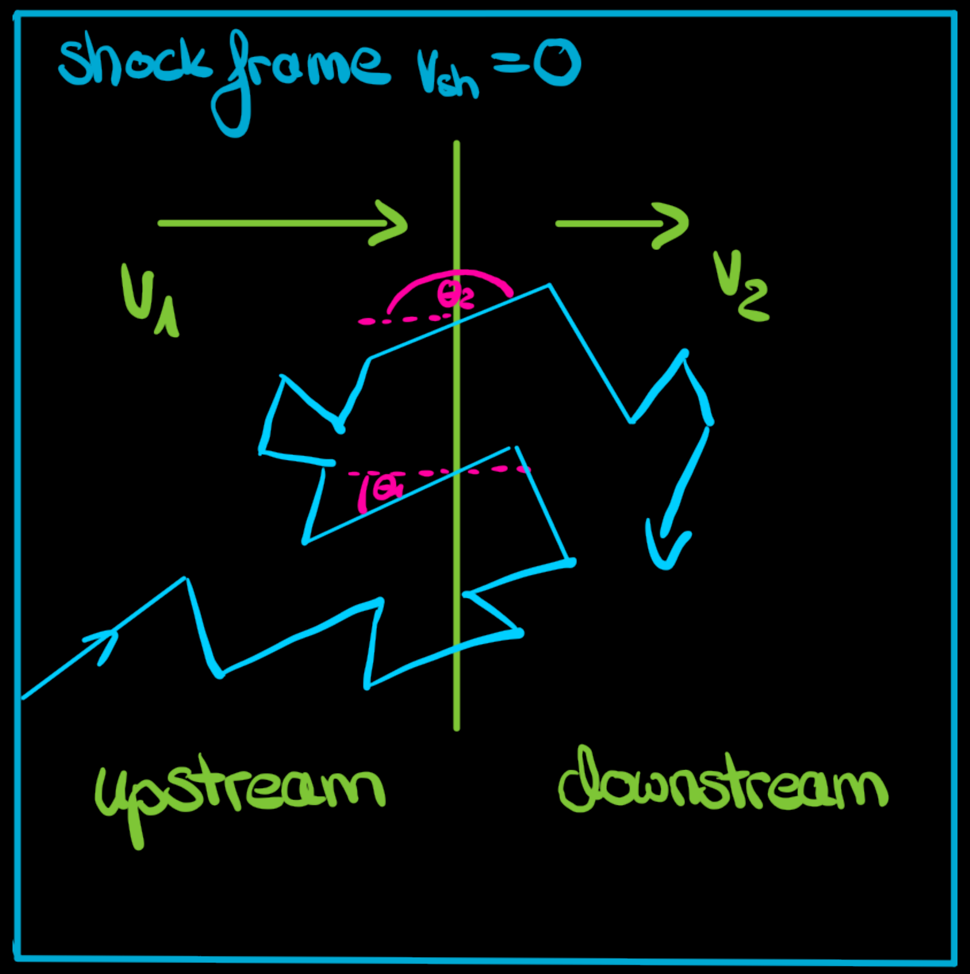


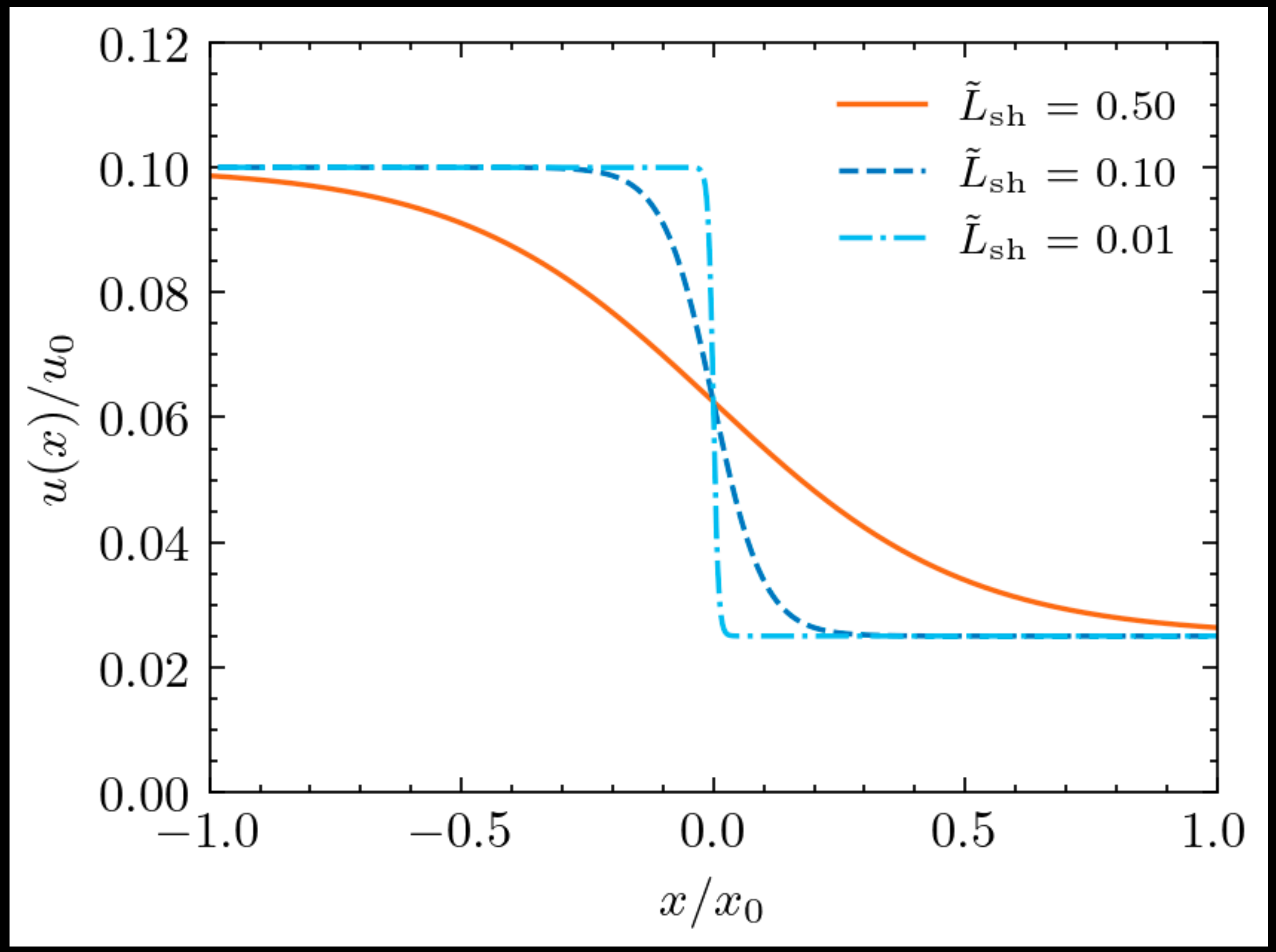
PARTICLE ACCELERATION

DIFFUSIVE SHOCK ACCELERATION

$$\mathrm{d}x = u(x)\mathrm{d}t + \sqrt{2\kappa}\,\mathrm{d}W_{x,t}$$

$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial x}\mathrm{d}t$$





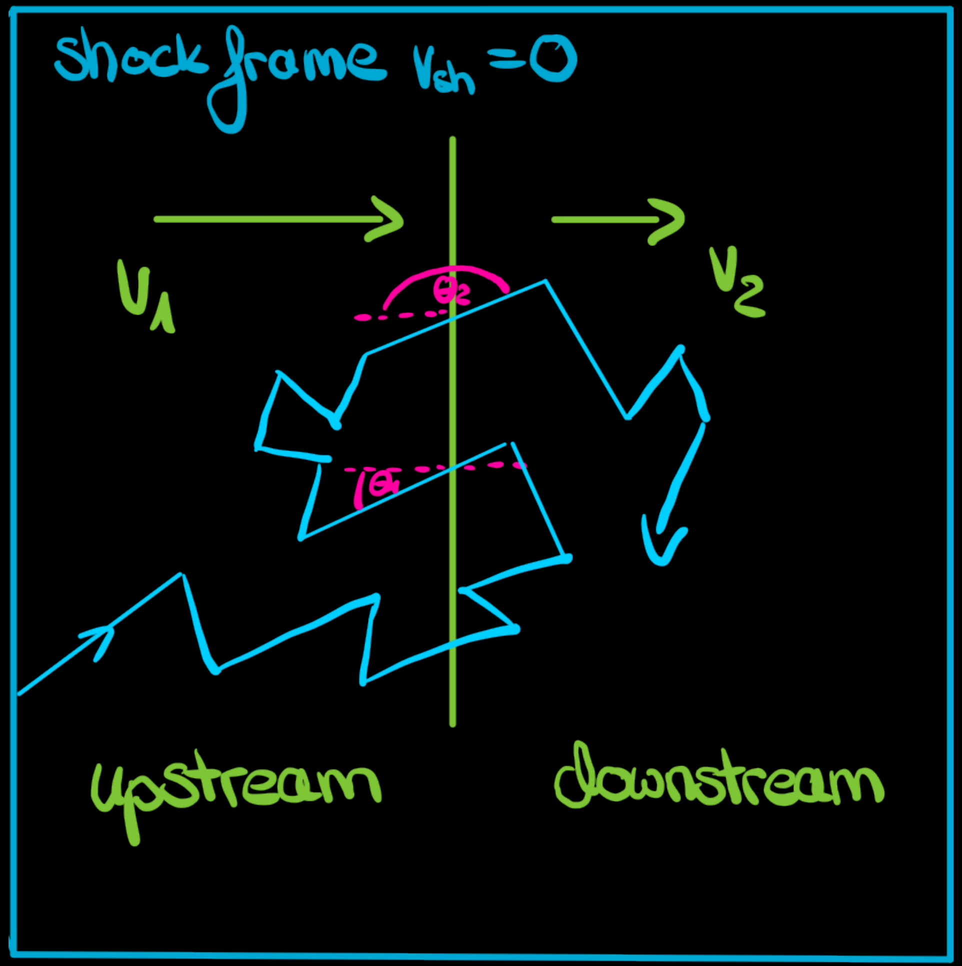
SA, et al., JCAP

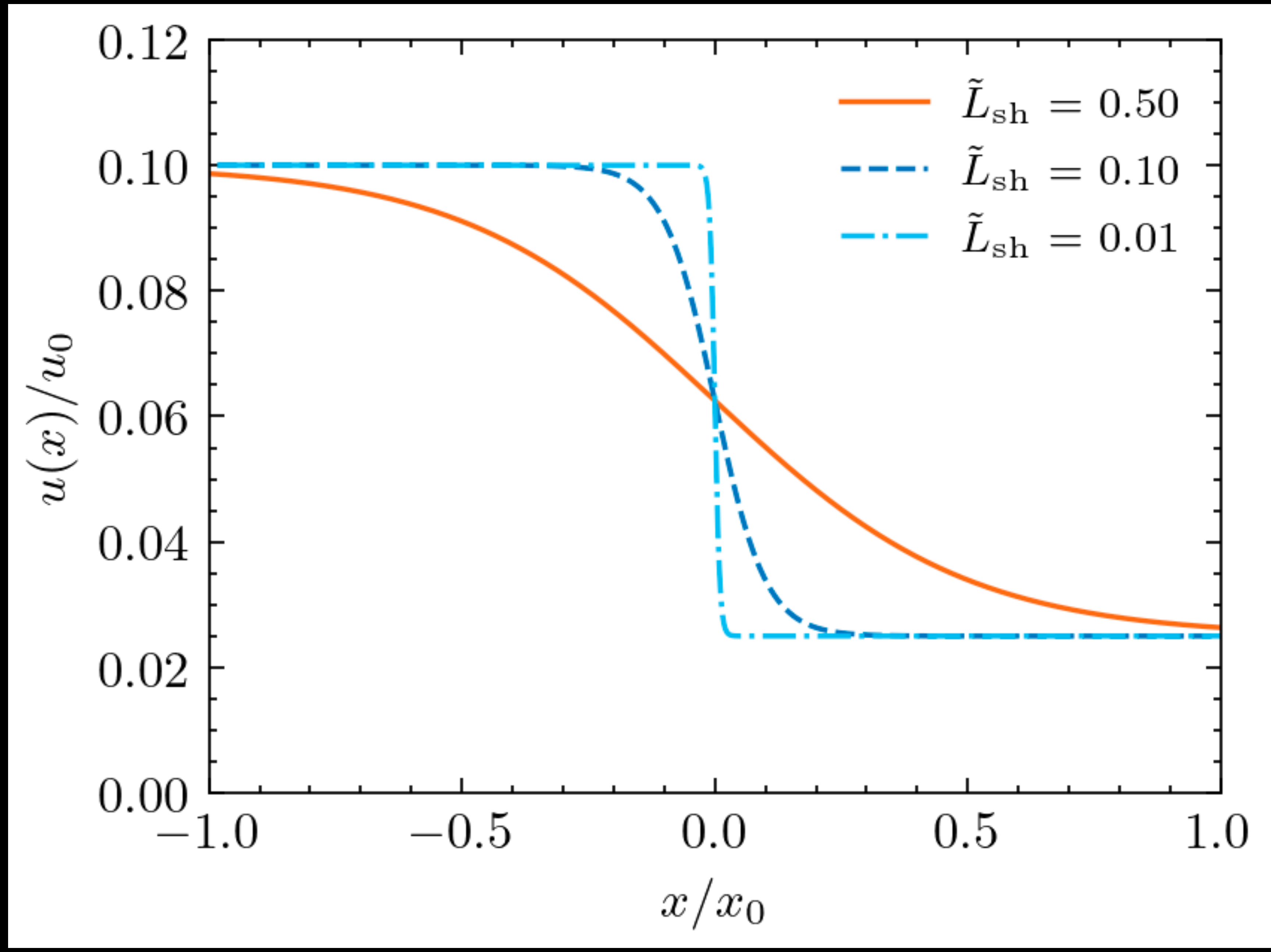
PARTICLE ACCELERATION

DIFFUSIVE SHOCK ACCELERATION

$$\mathrm{d}x = u(x)\mathrm{d}t + \sqrt{2\kappa}\,\mathrm{d}W_{x,t}$$ ← SDE

$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial x}\mathrm{d}t$$ ← ODE

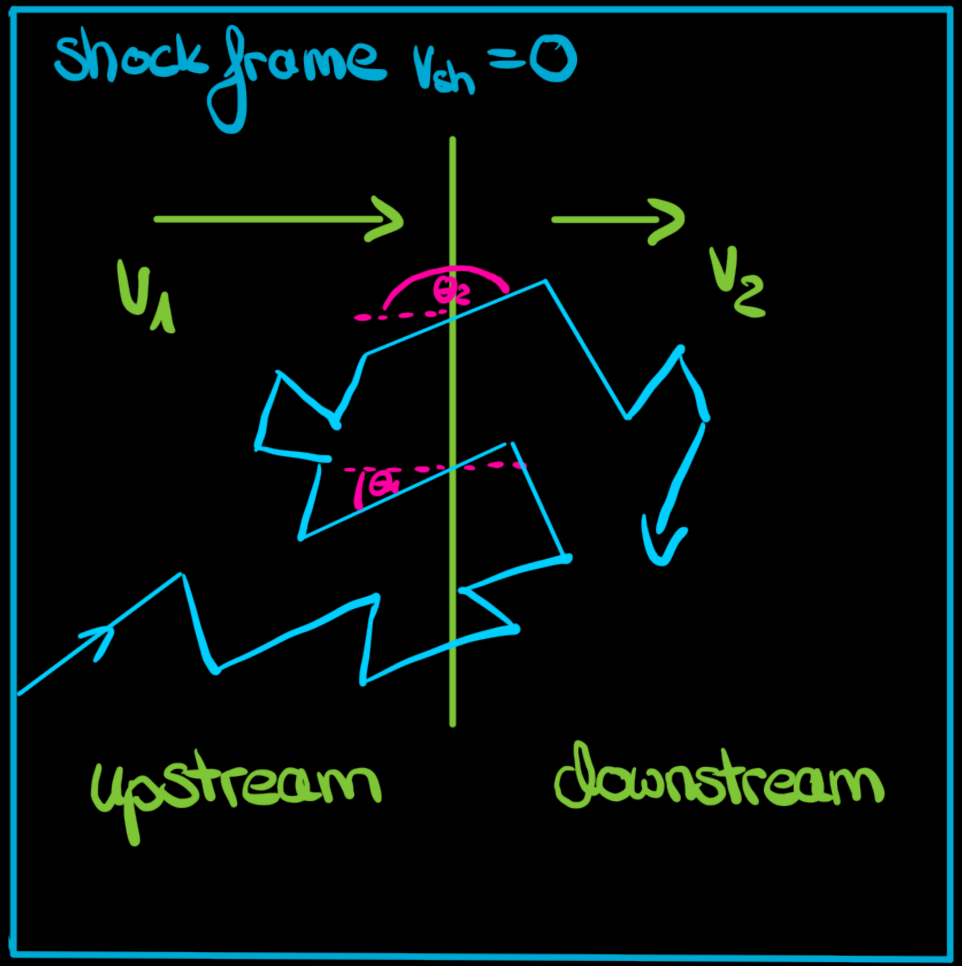




SA, et al., JCAP

PARTICLE ACCELERATION

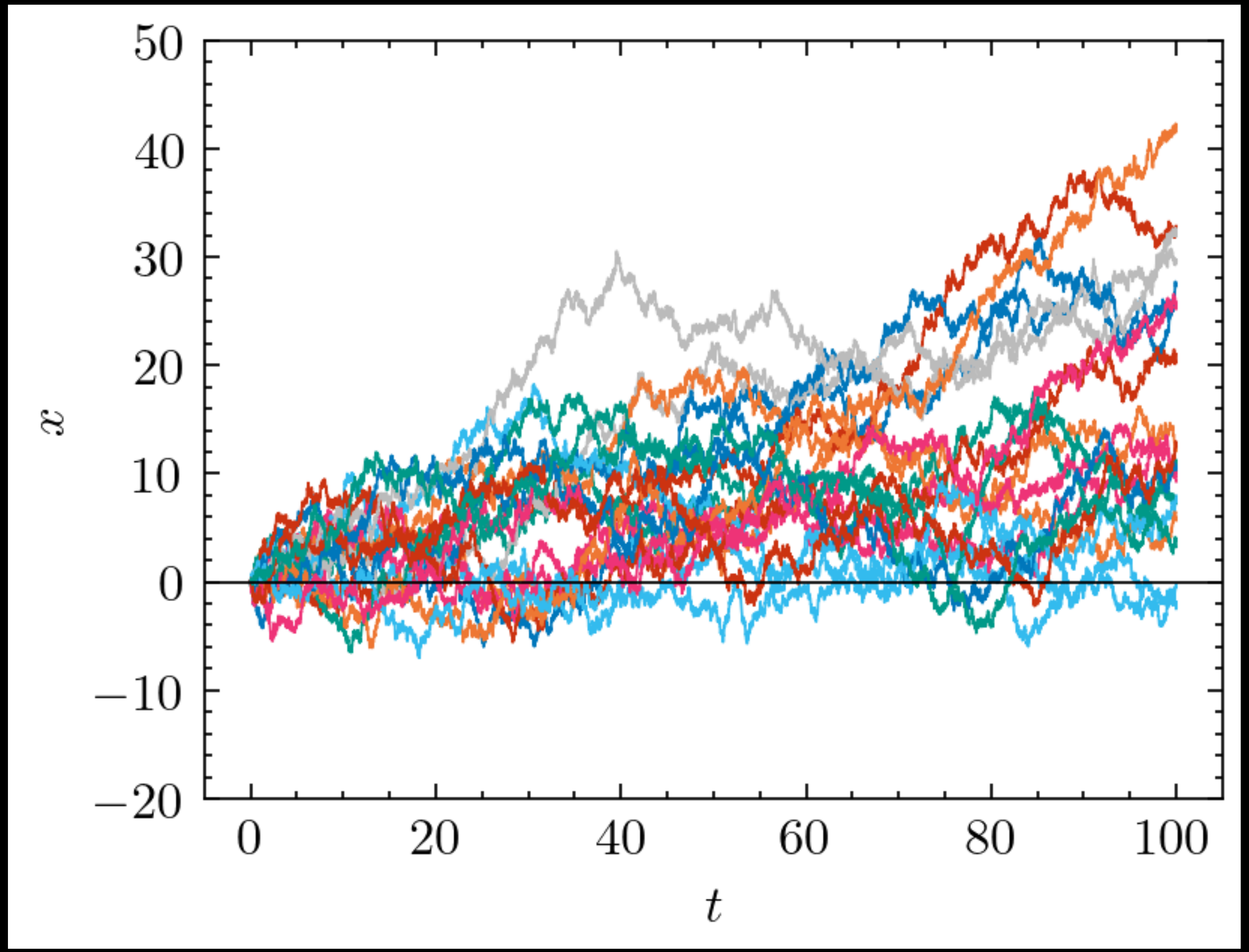
DIFFUSIVE SHOCK ACCELERATION



$$\mathrm{d}x = u(x)\mathrm{d}t + \sqrt{2\kappa}\,\mathrm{d}W_{x,t}$$

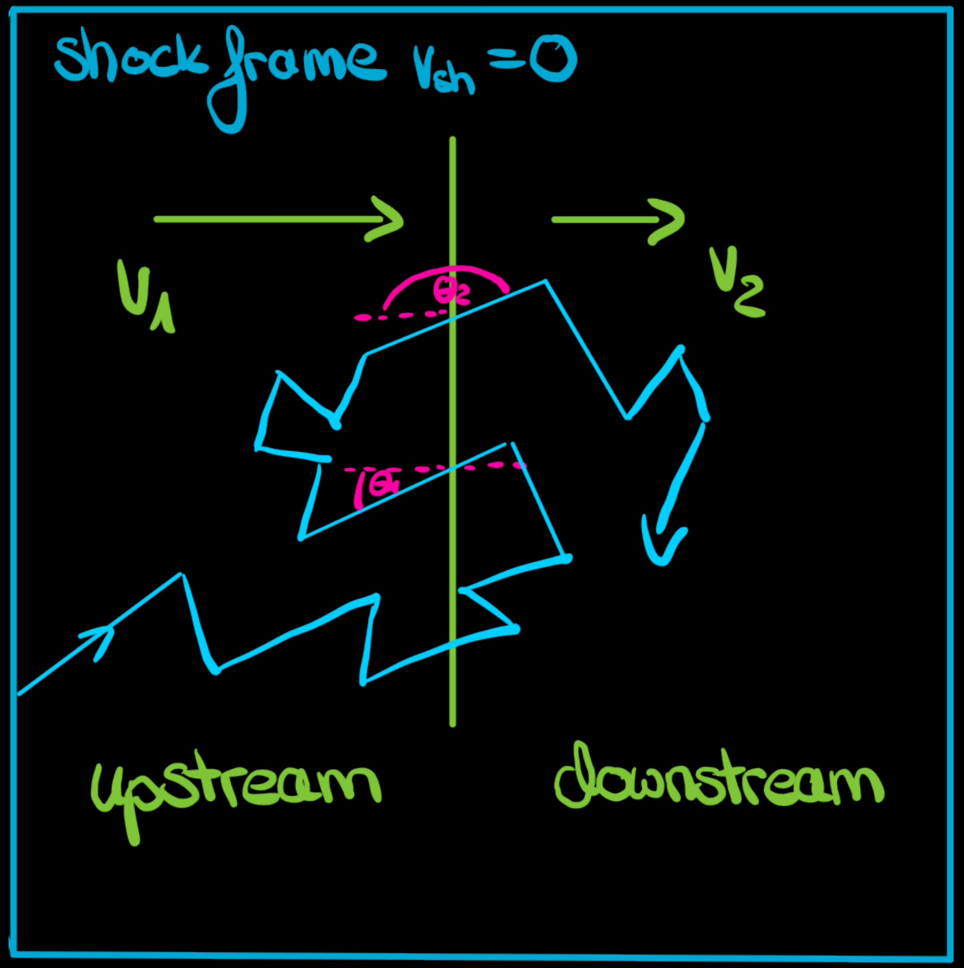
$$u\Delta t < L_{\mathrm{sh}} \lesssim \sqrt{2\kappa\Delta t}$$

$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial x}\mathrm{d}t$$



PARTICLE ACCELERATION

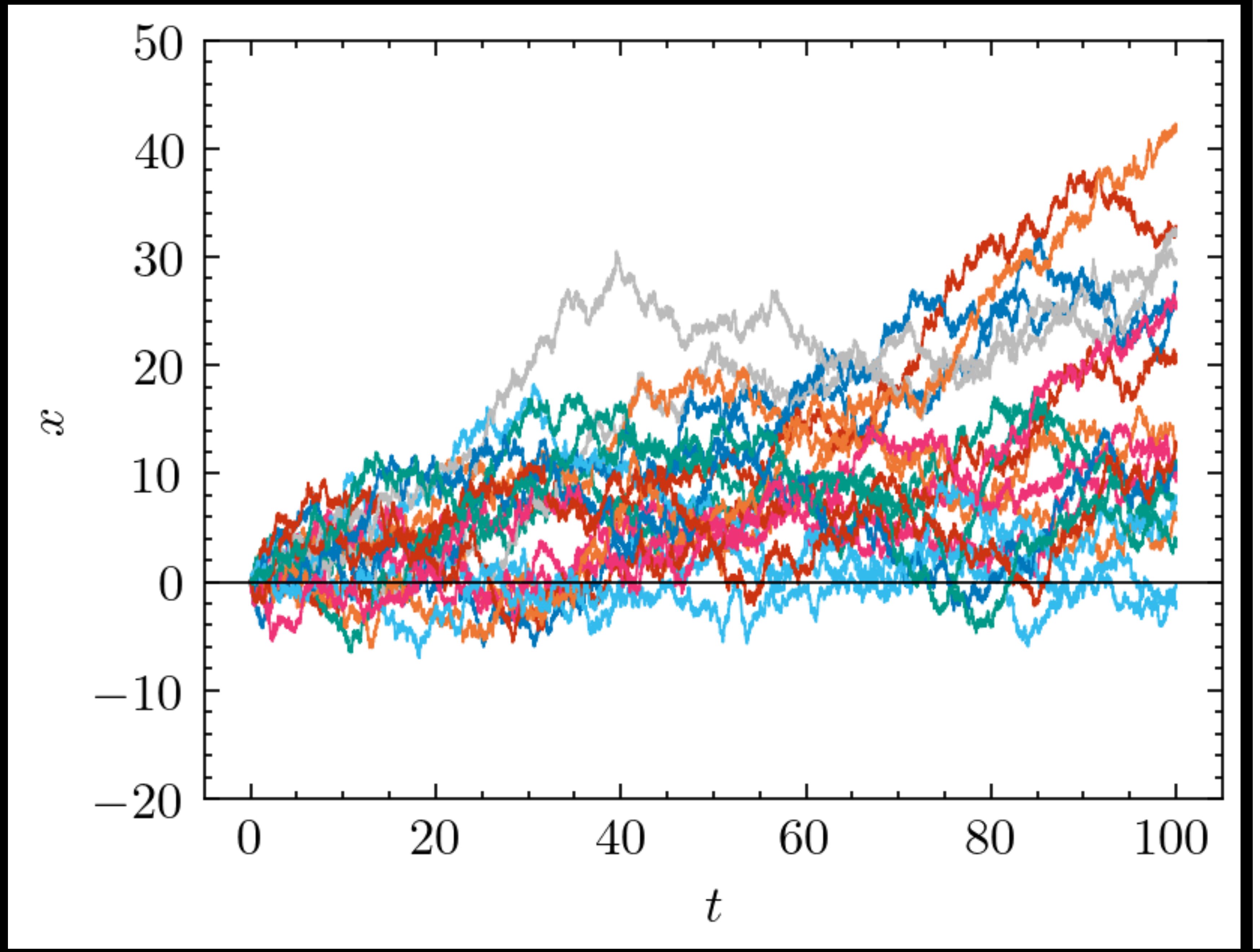
DIFFUSIVE SHOCK ACCELERATION

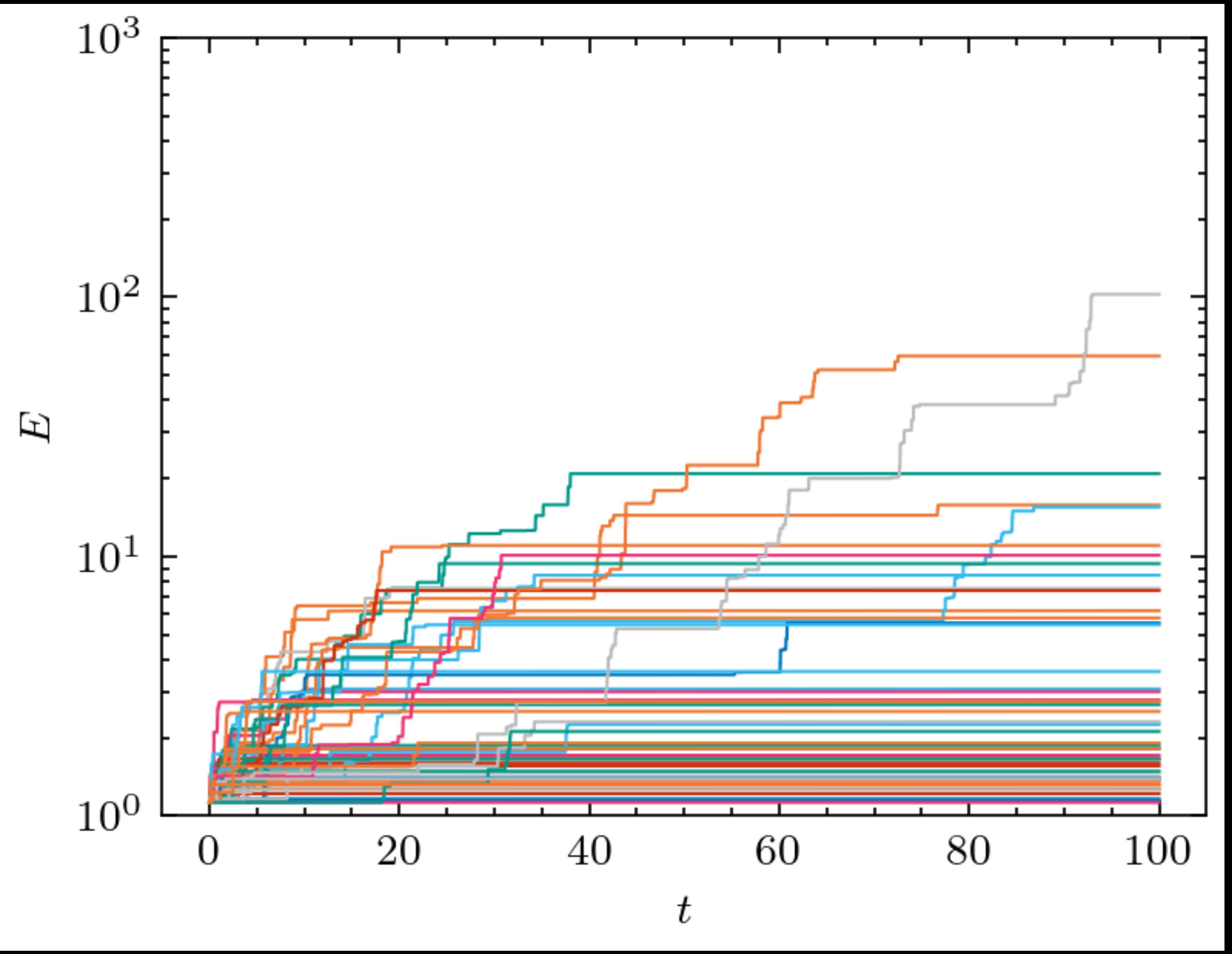


$$\mathrm{d}x = u(x)\mathrm{d}t + \sqrt{2\kappa}\,\mathrm{d}W_{x,t}$$

$$u\Delta t < L_{\mathrm{sh}} \lesssim \sqrt{2\kappa\Delta t}$$

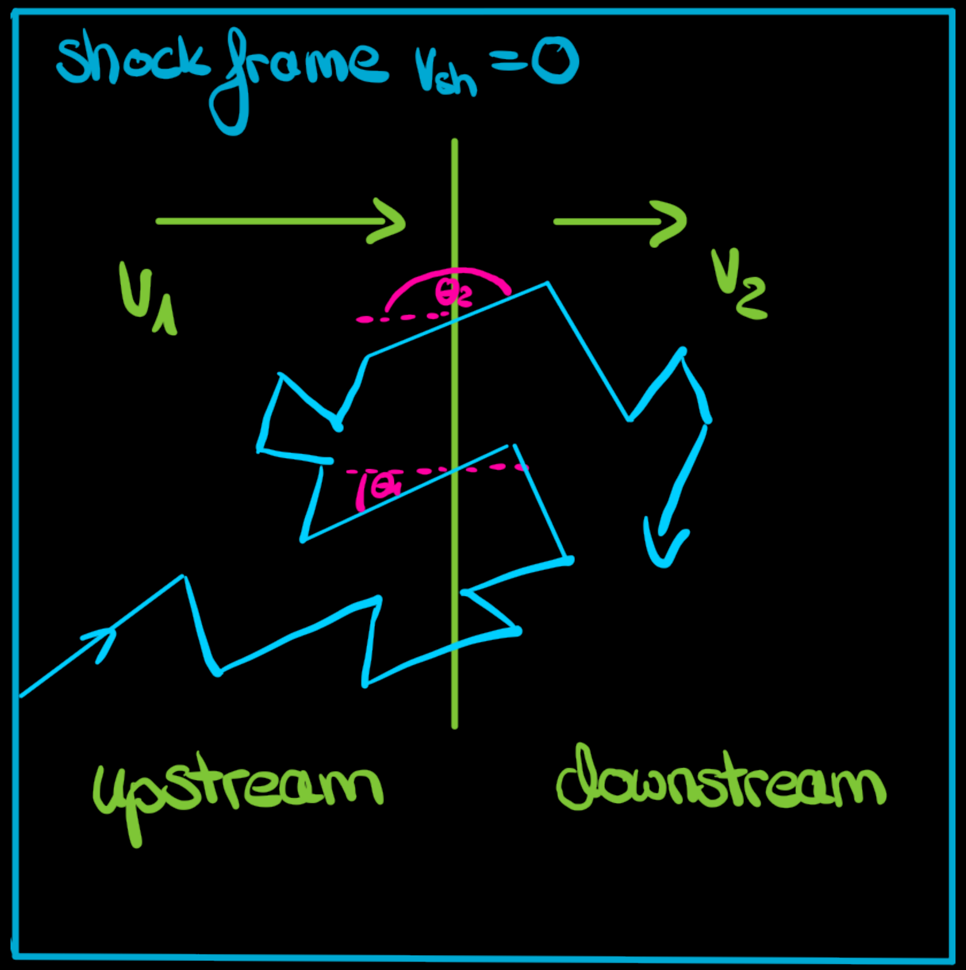
$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial x}\mathrm{d}t$$





PARTICLE ACCELERATION

DIFFUSIVE SHOCK ACCELERATION



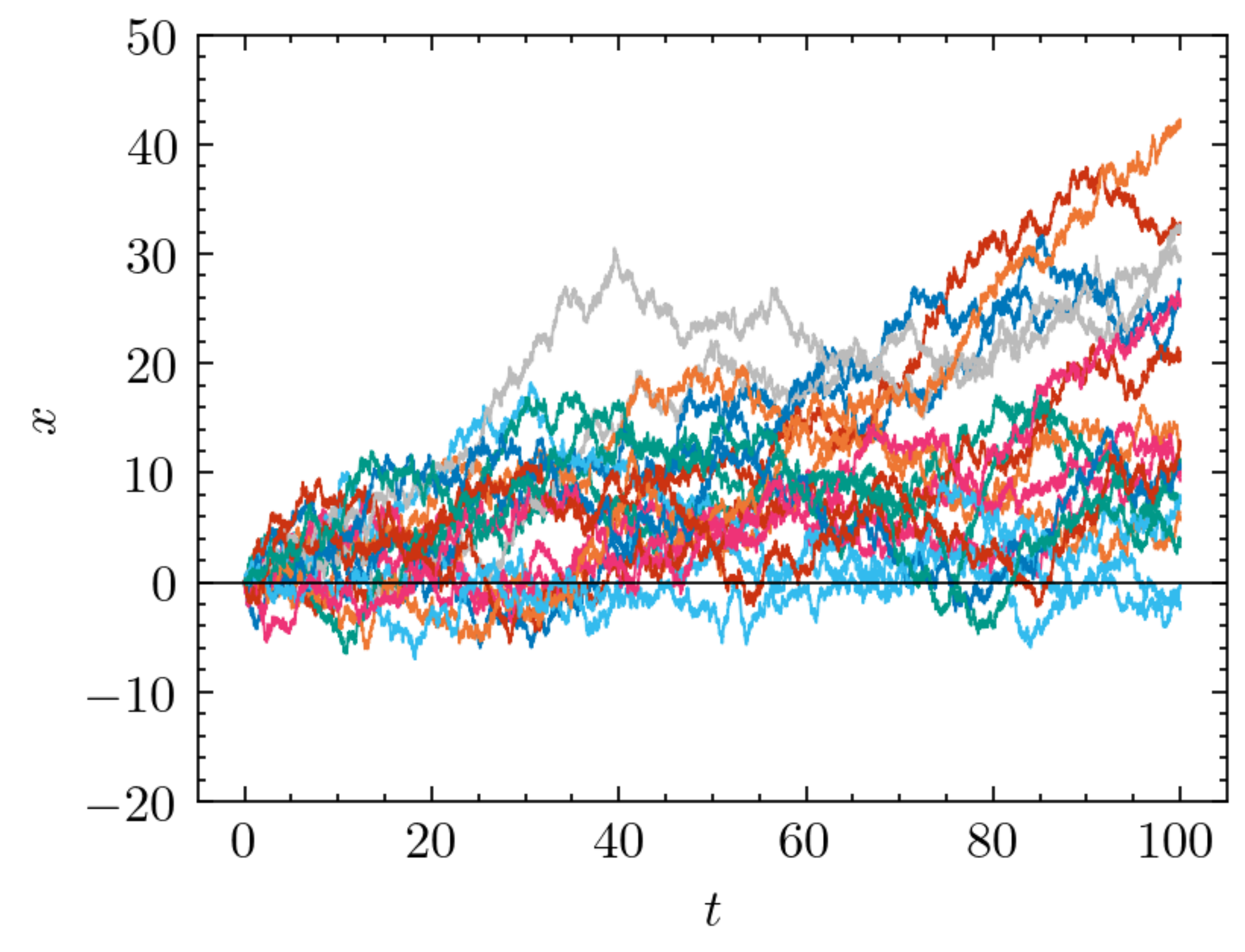
$$\mathrm{d}x = u(x)\mathrm{d}t + \sqrt{2\kappa}\,\mathrm{d}W_{x,t}$$

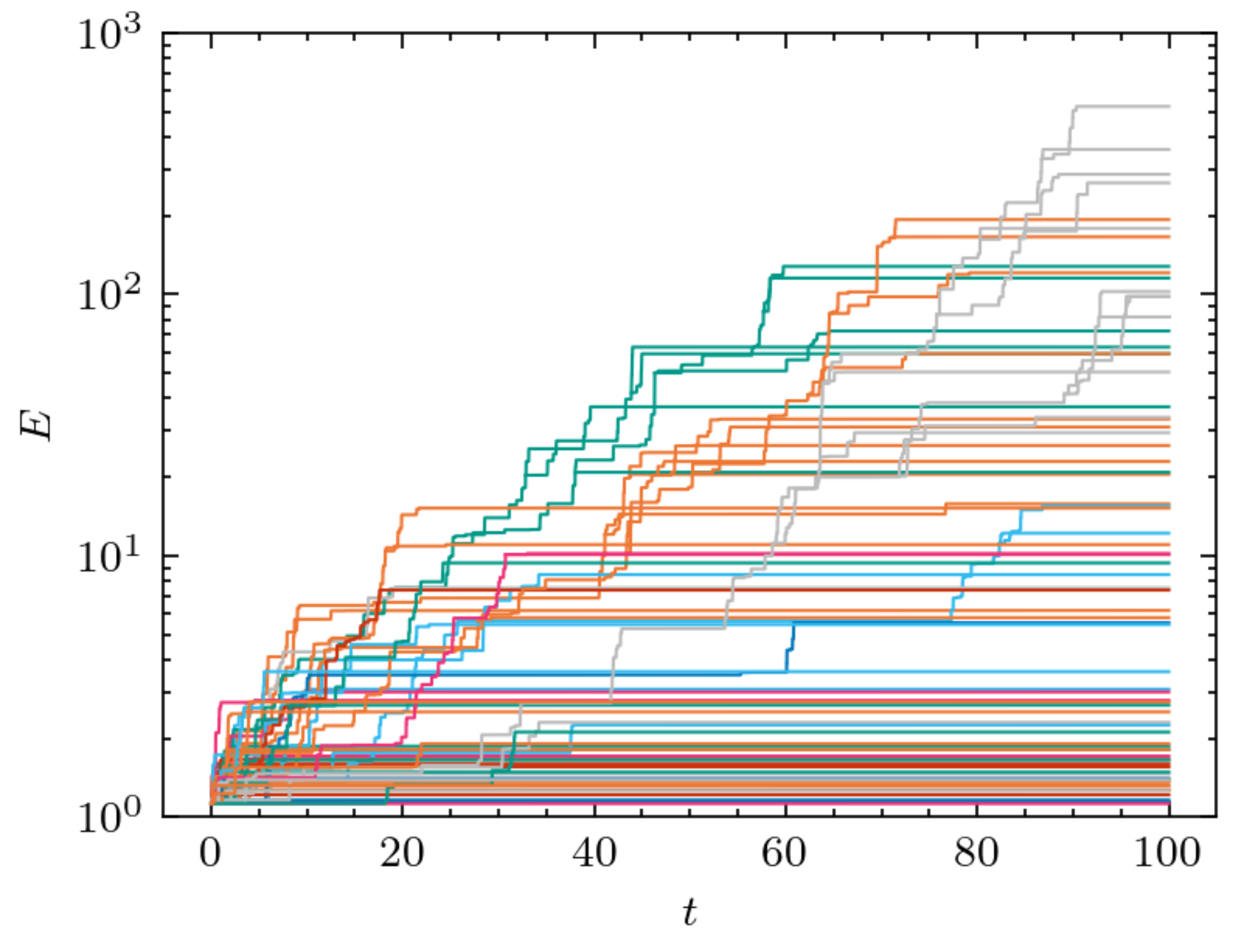
$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial x}\mathrm{d}t$$

$$u\Delta t < L_{\mathrm{sh}} \lesssim \sqrt{2\kappa\Delta t}$$

$$w_i = 1/n_{\mathrm{split}}$$

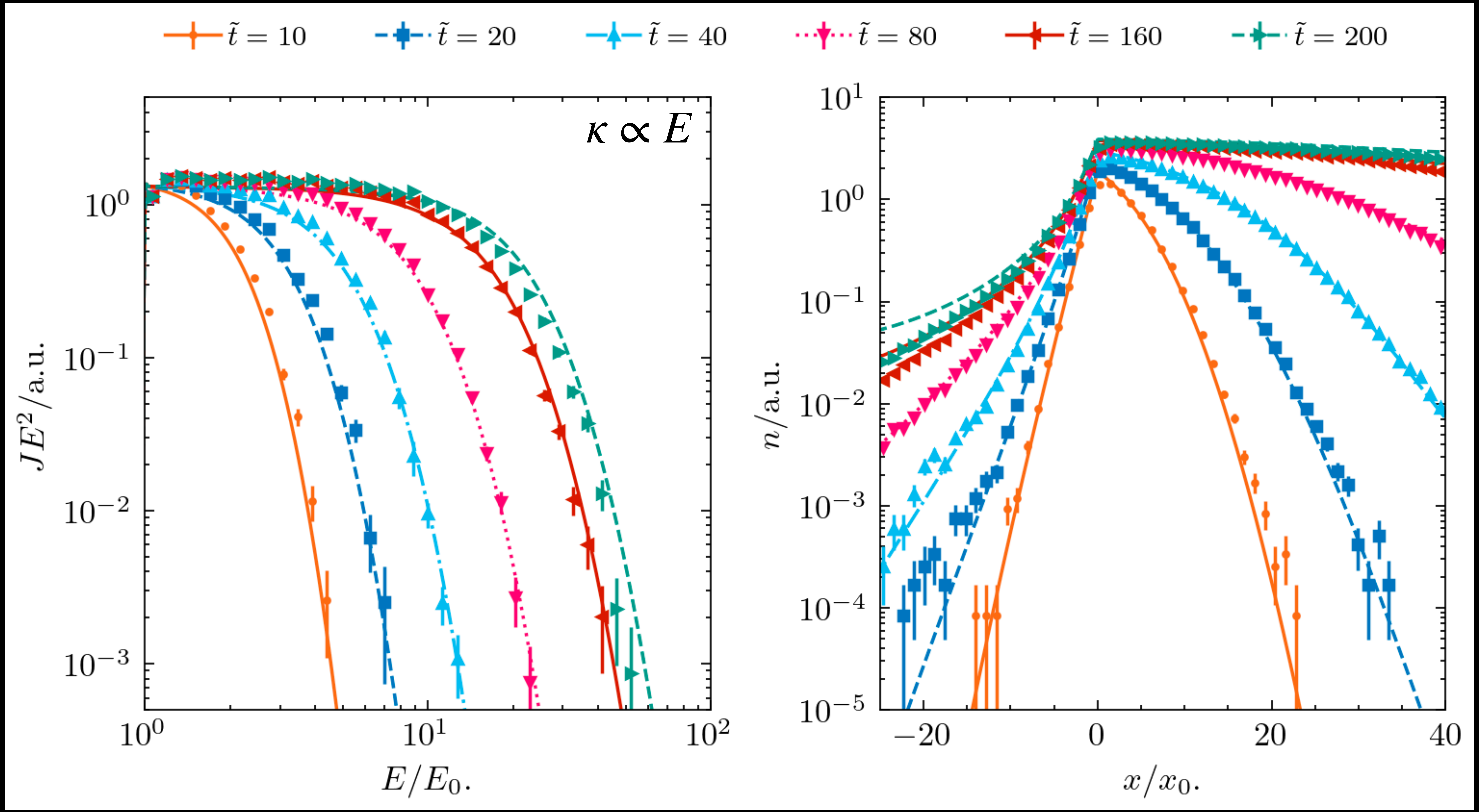
- Importance sampling

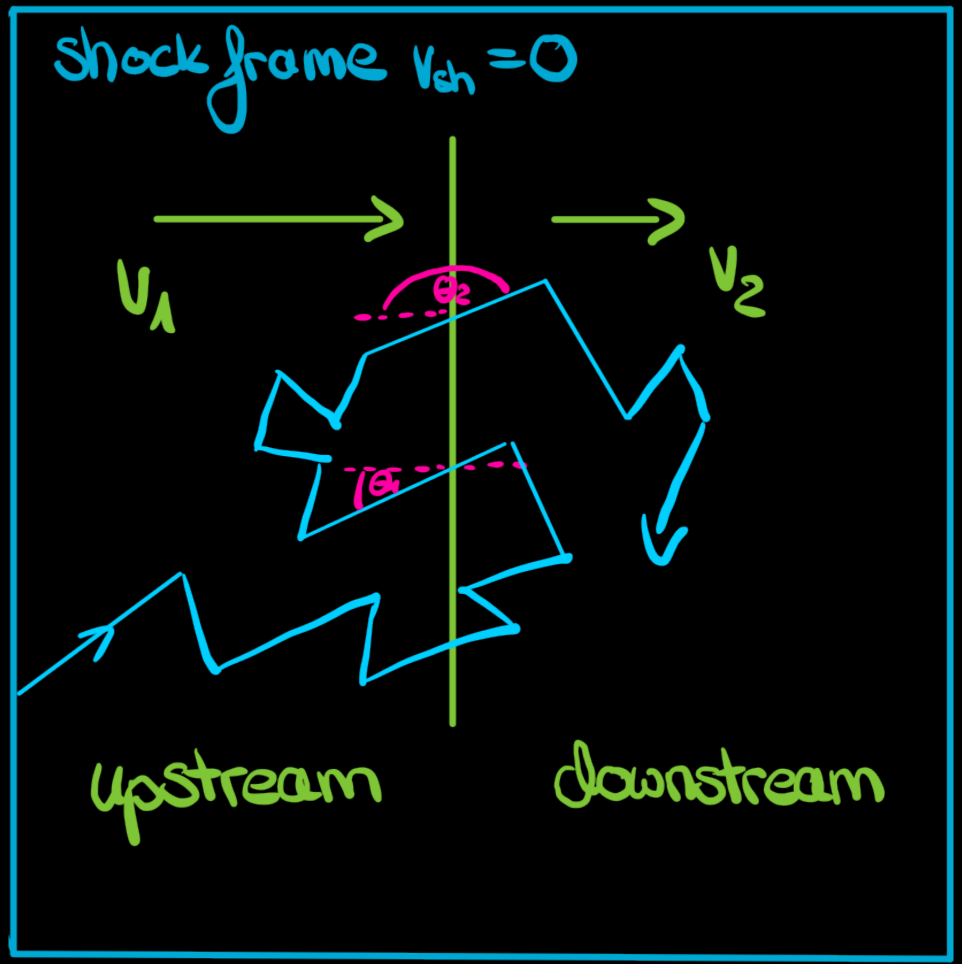




TIME-DEPENDENT SPECTRA

DSA AT 1D PLANAR SHOCK



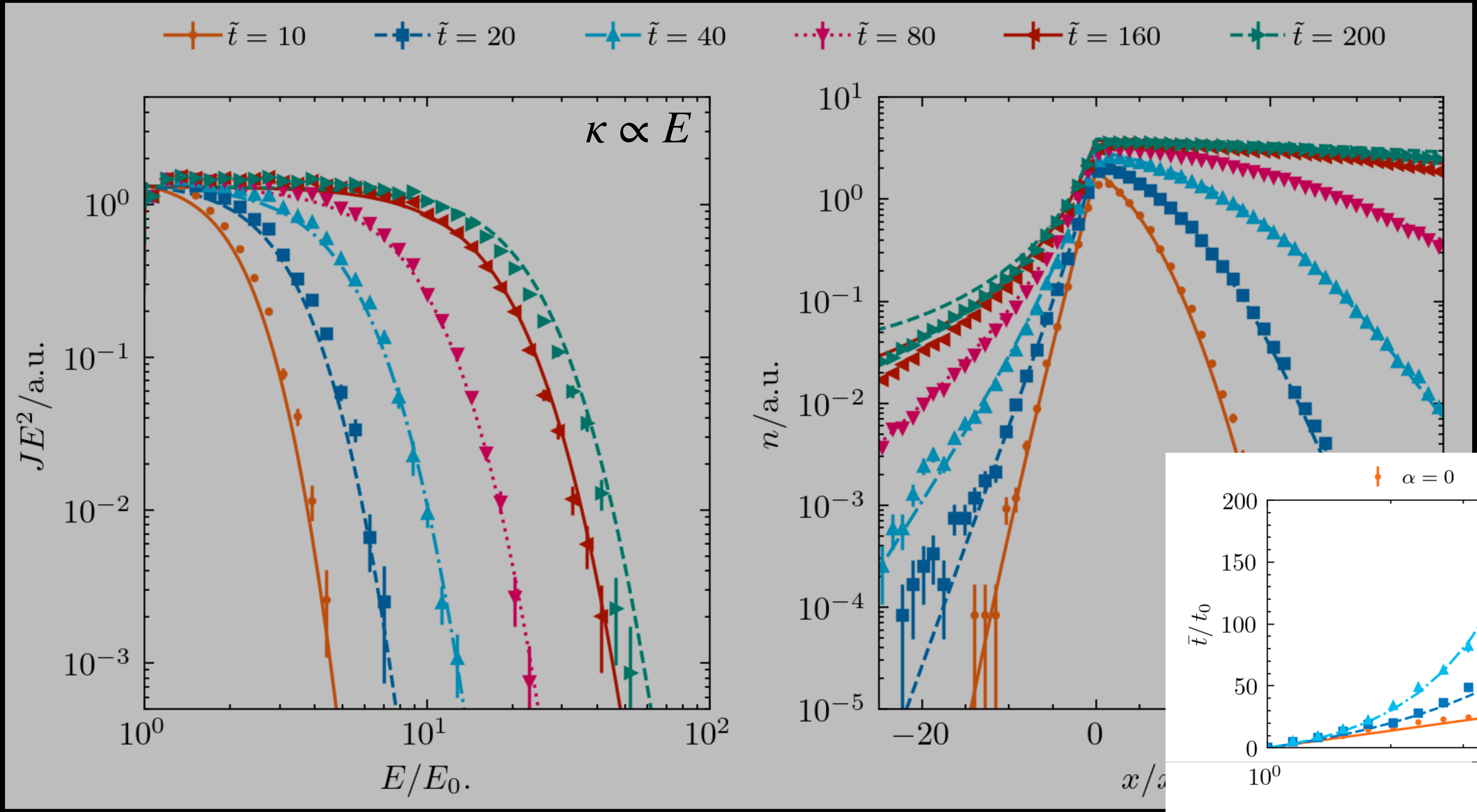


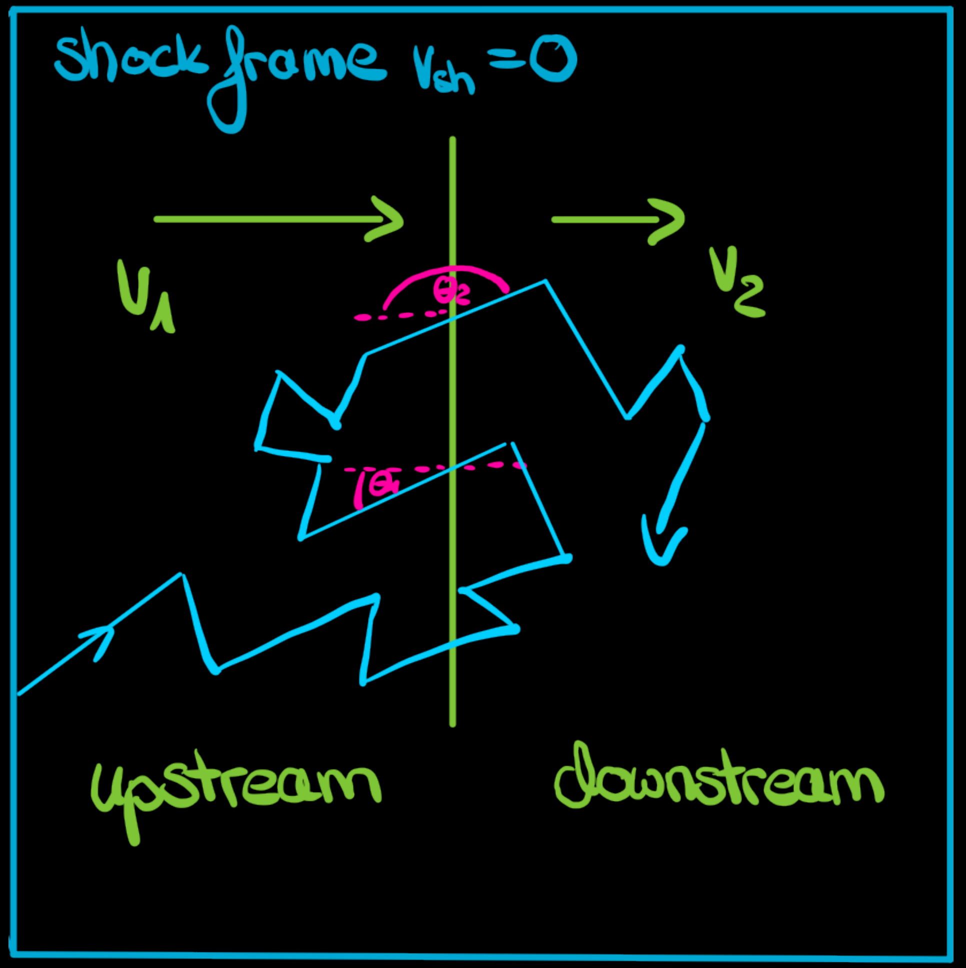
- Validation: Comparison against grid code VLUGR3 solving the transport equation

SA, et al., JCAP (2024)

TIME-DEPENDENT SPECTRA

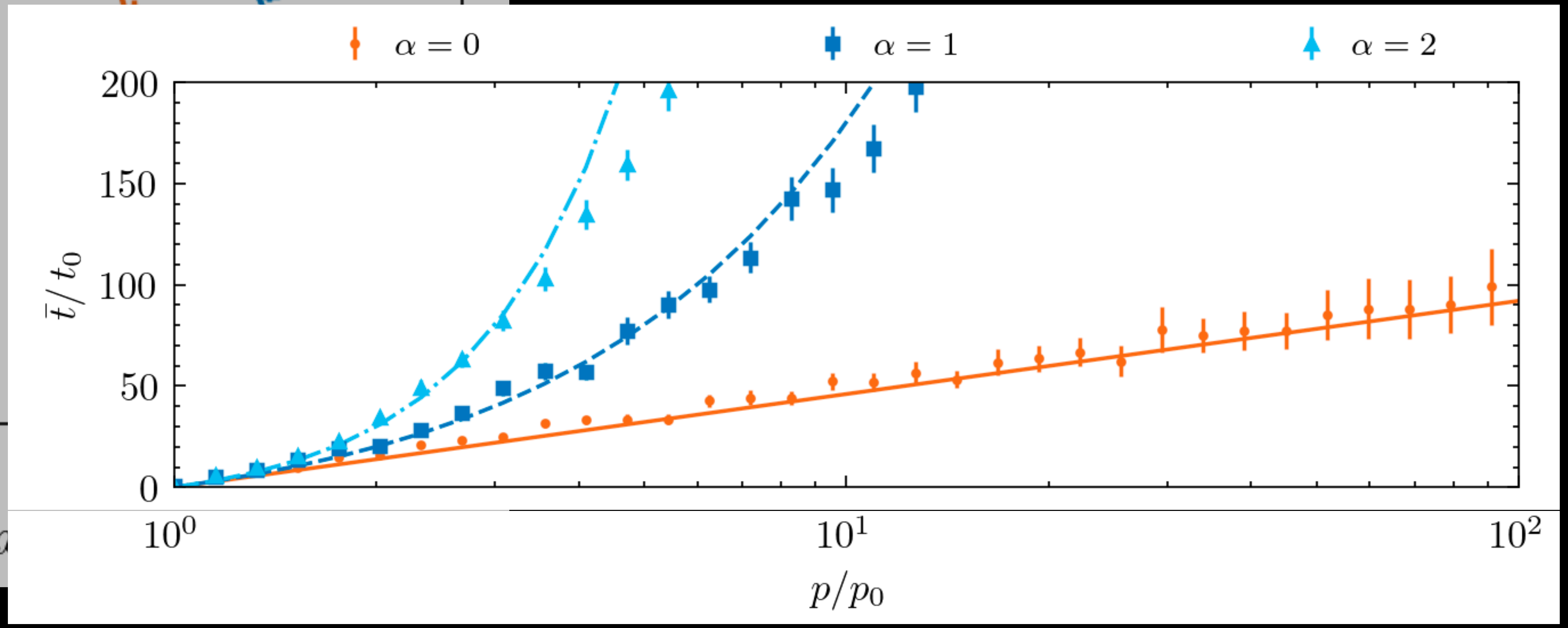
DSA AT 1D PLANAR SHOCK





- Validation: Comparison against grid code VLUGR3 solving the transport equation

$\kappa \propto p^\alpha$

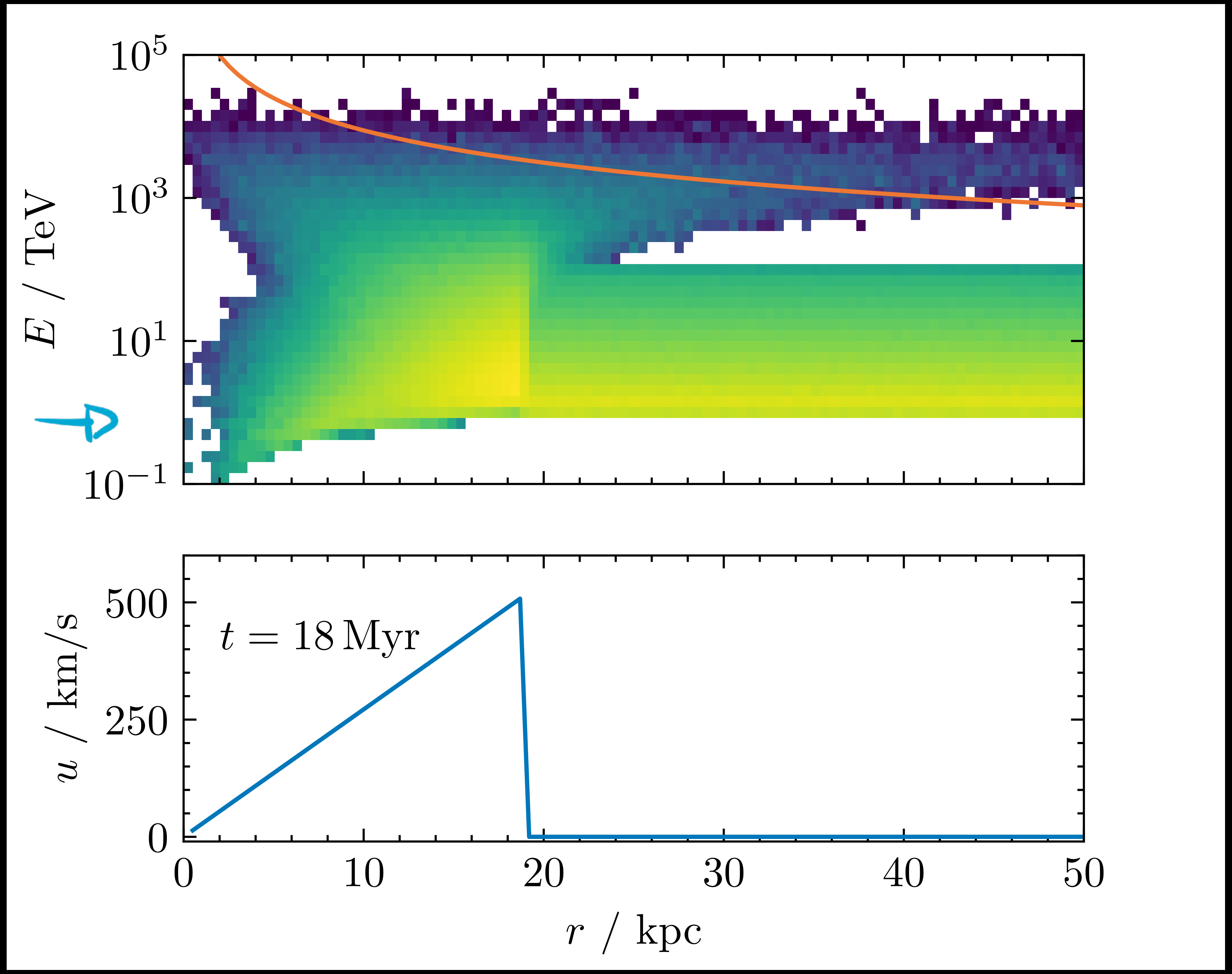


MOVING SHOCKS

SPHERICAL BLAST WAVES

- Blast wave moving out into medium with decreasing density (Isenberg, 1977)
- Bohm diffusion coefficient, $B \propto r^{-2}$
- Spectrum between knee and ankle?

pre-accelerated spectrum $\sim E^{-2}$



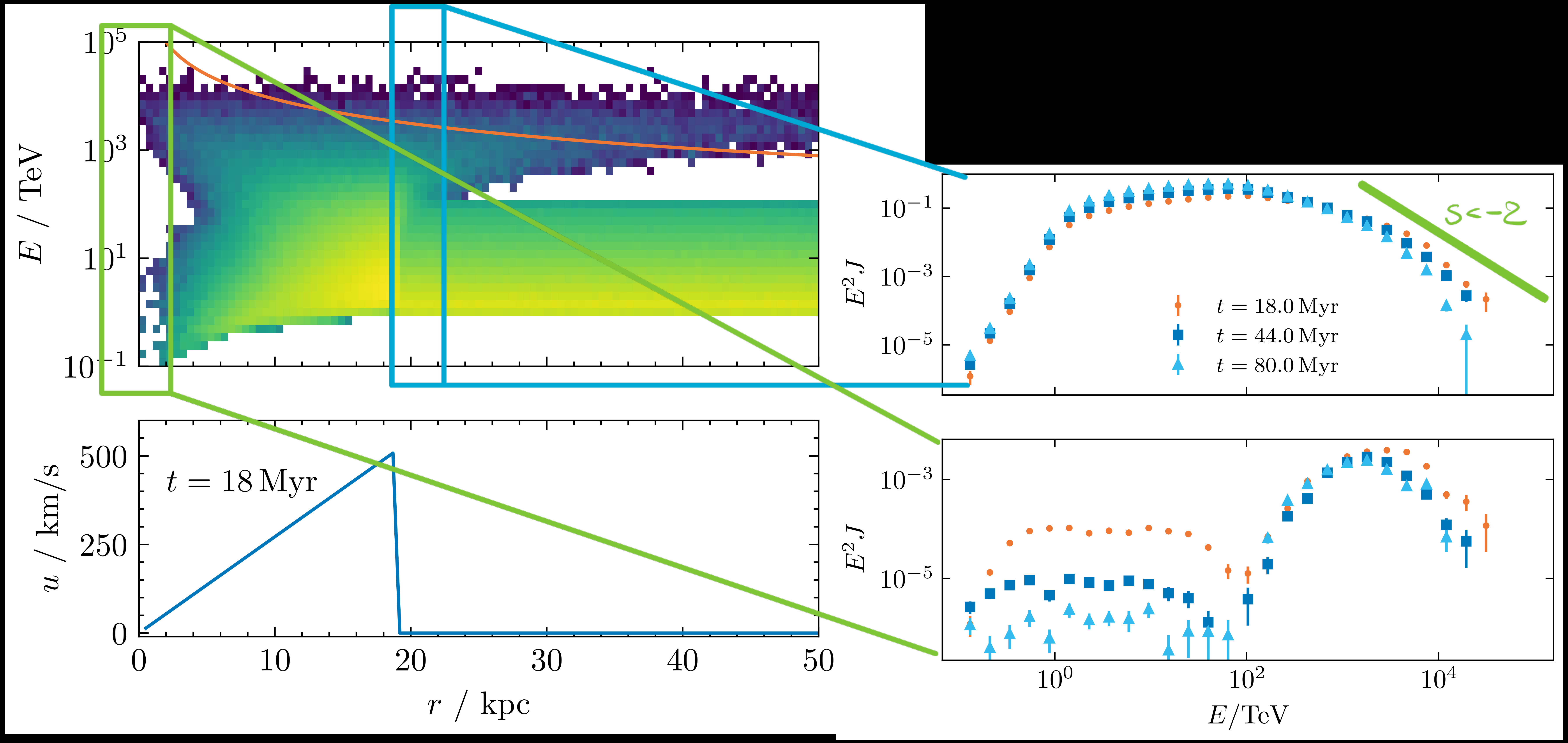
injected upstream of shock

$$\mathrm{d}r = \left(\frac{\partial\kappa}{\partial r} + u(t,r)\right)\mathrm{d}t + \sqrt{2\kappa(p,r)}\,\mathrm{d}W_{r,t}$$

$$\mathrm{d}p = -\frac{p}{3}\frac{\partial u}{\partial r}\,\mathrm{d}t$$

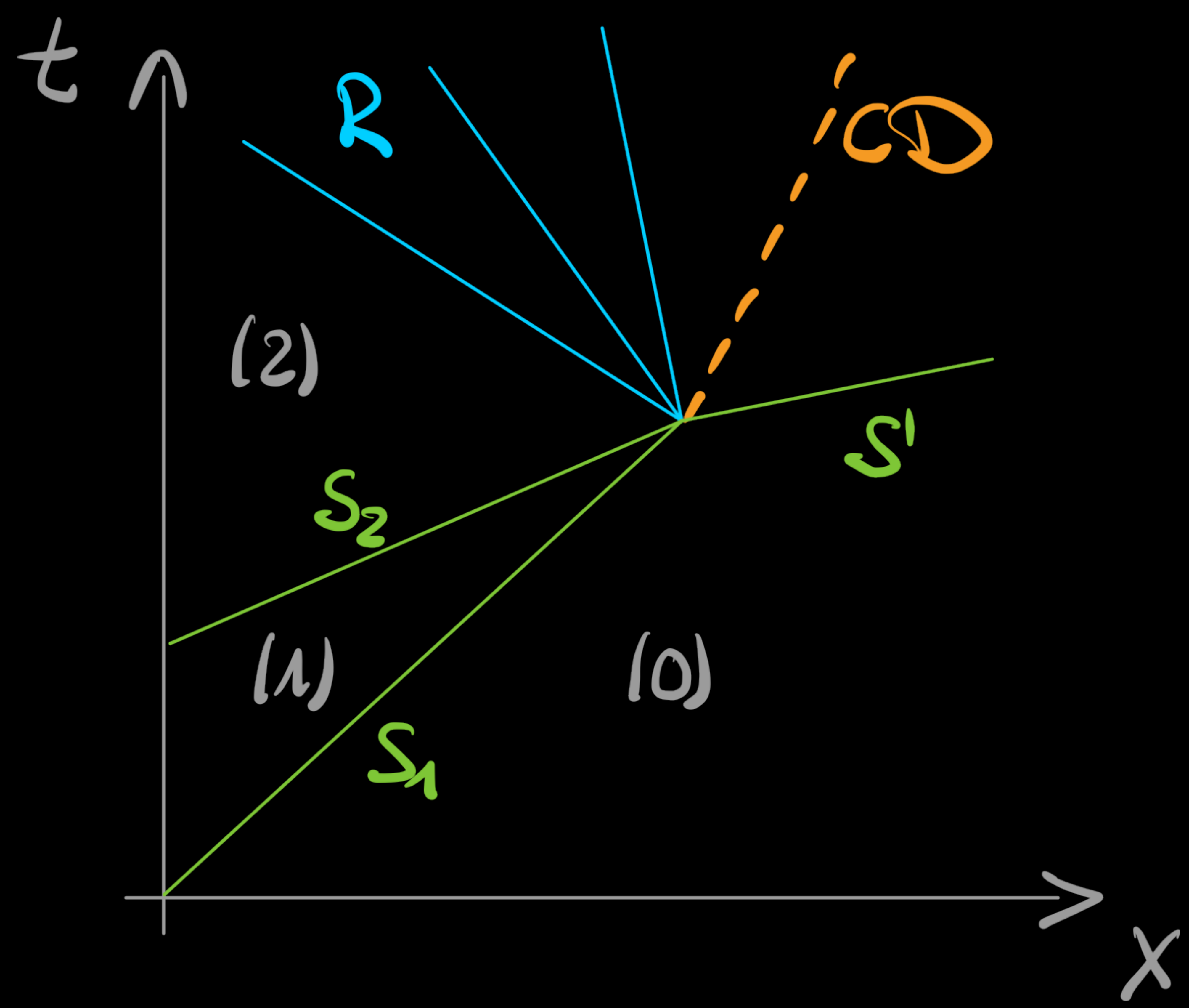
MOVING SHOCKS

SPHERICAL BLAST WAVES



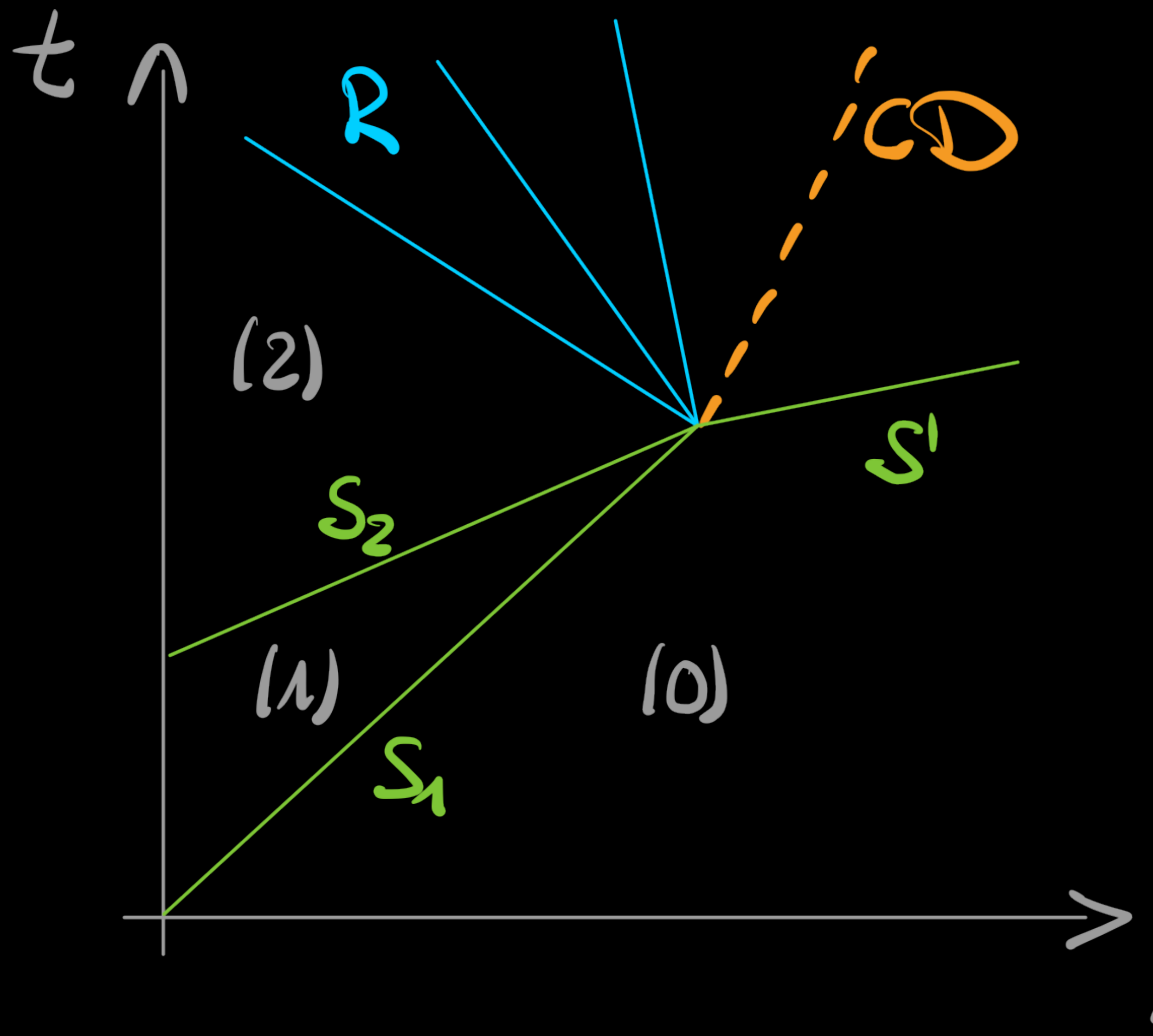
COLLIDING SHOCKS

CATCHING UP WITH EACH OTHER

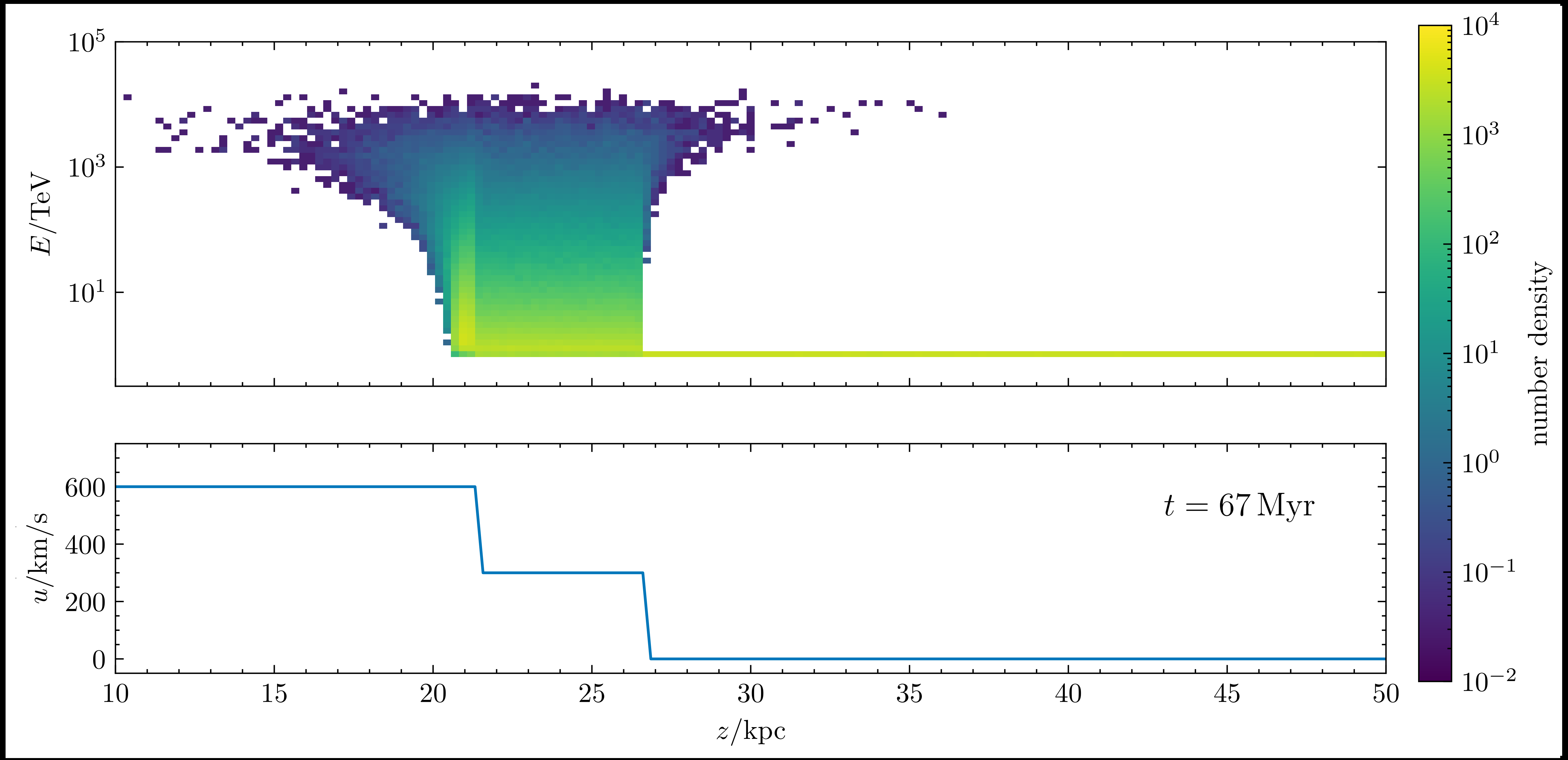


COLLIDING SHOCKS

CATCHING UP WITH EACH OTHER



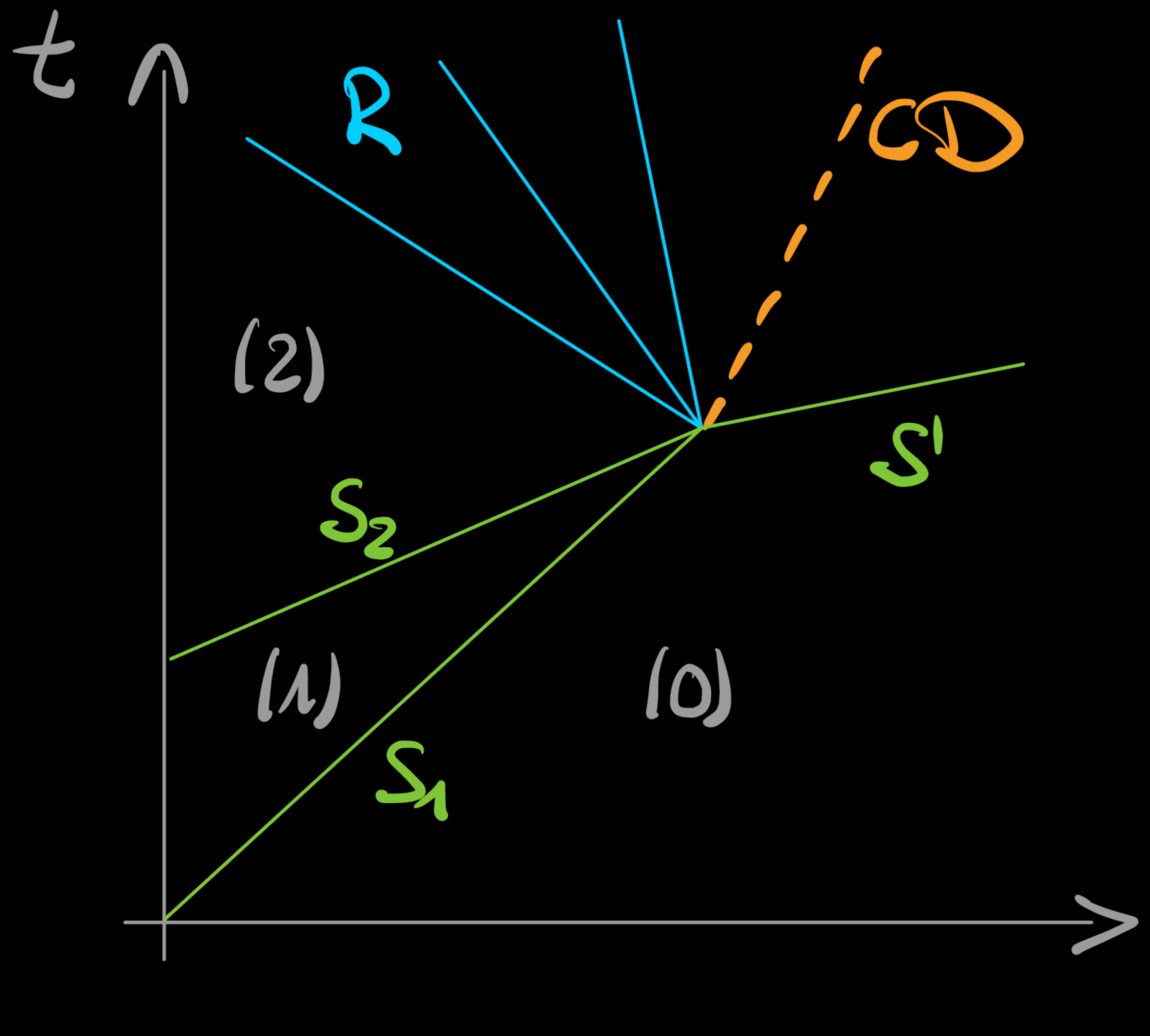
mono-energetic



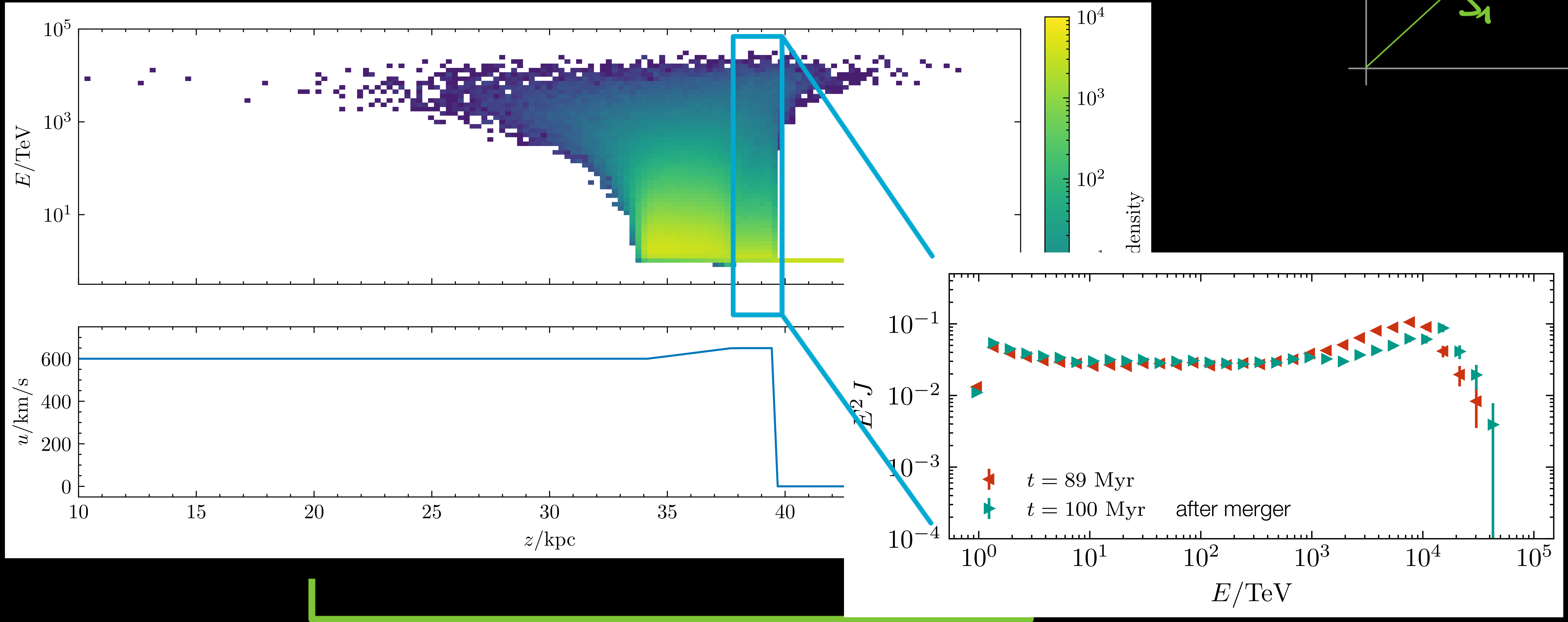
injected upstream of shock

COLLIDING SHOCKS

CATCHING UP WITH EACH OTHER



mono-energetic

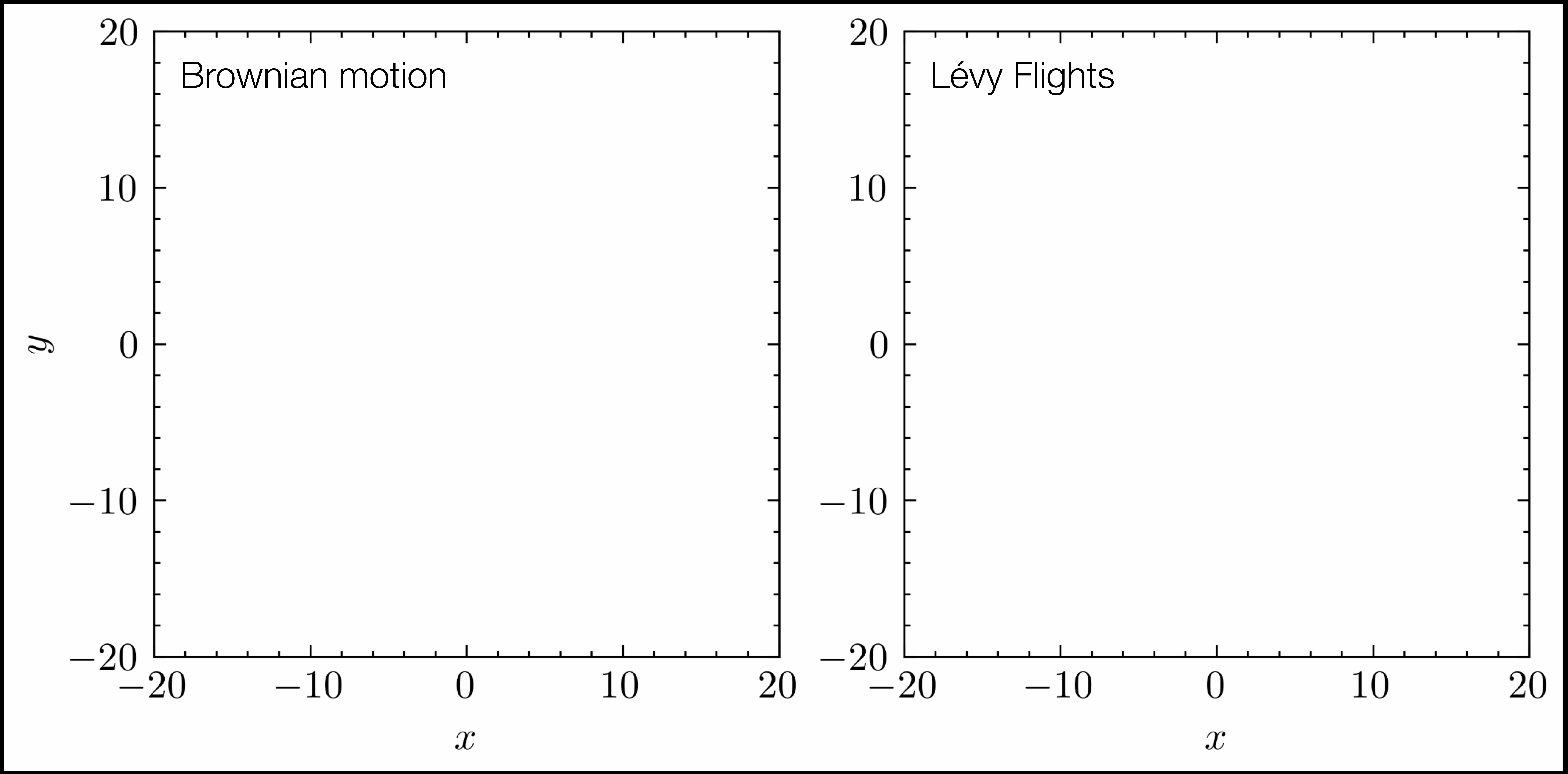


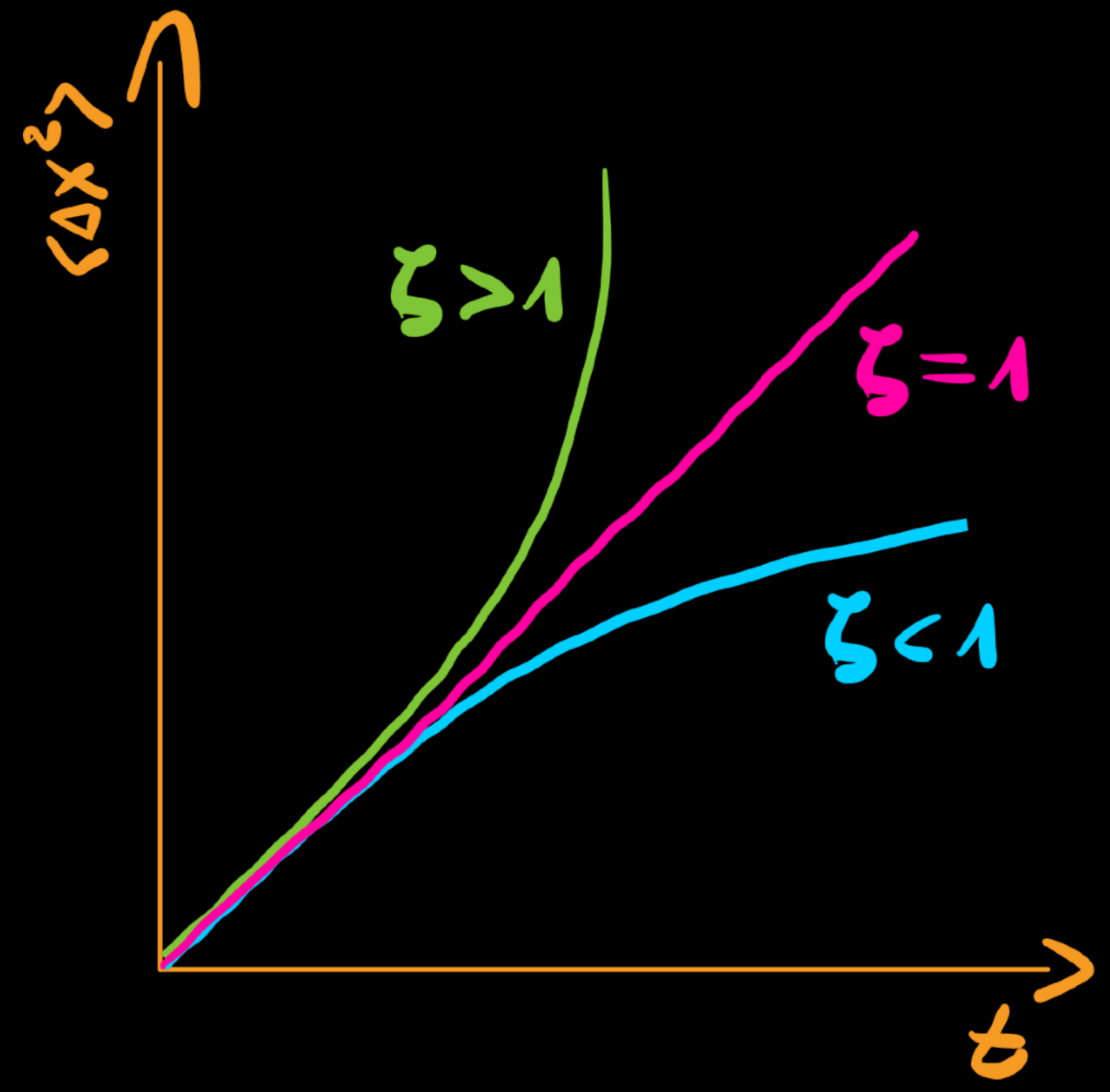
injected upstream of shock

ANOMALOUS DIFFUSION

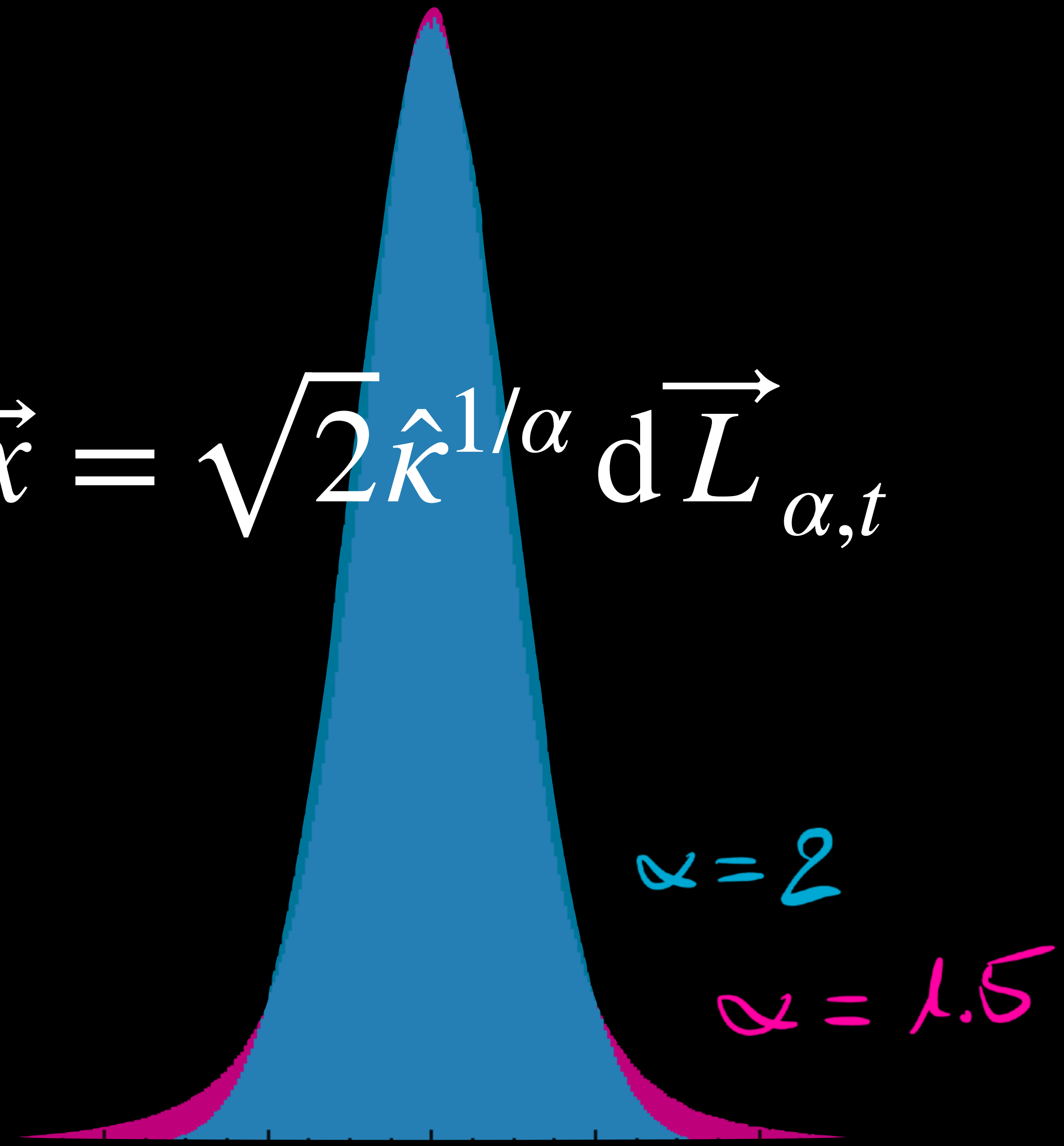
SUPERDIFFUSION

LEVY FLIGHTS



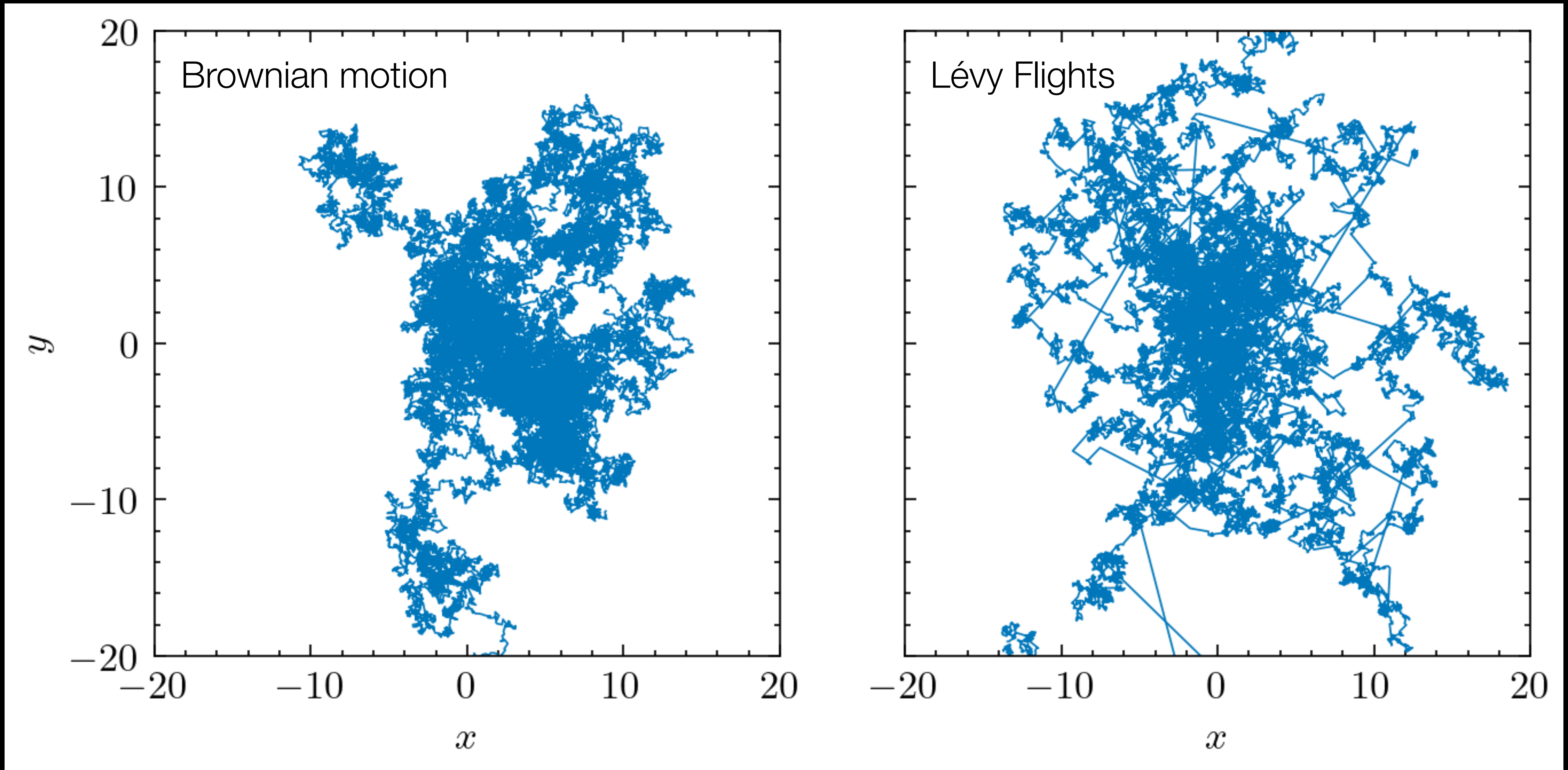


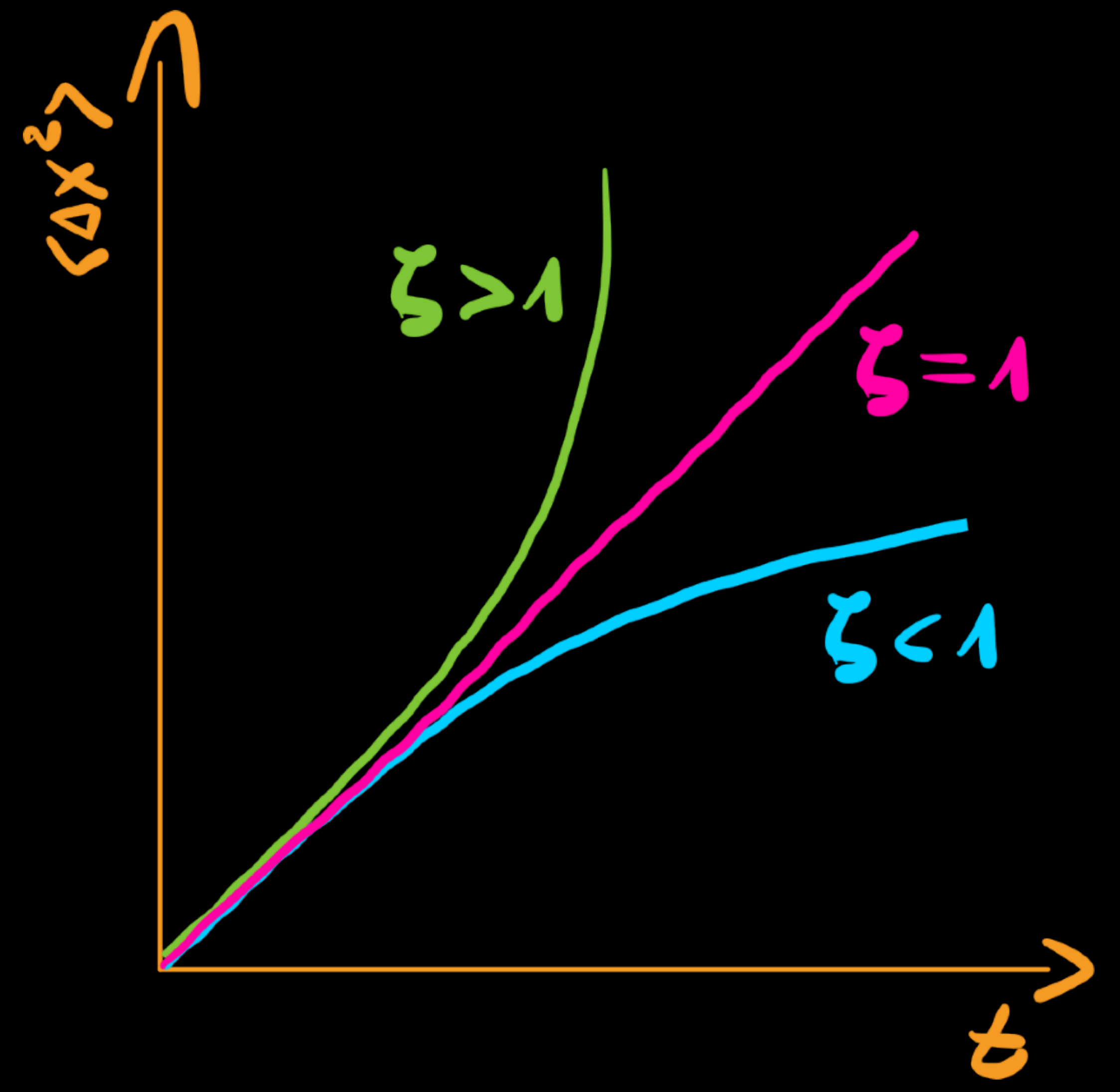
$$\mathrm{d}\vec{x} = \sqrt{2\hat{\kappa}^{1/\alpha}}\,\mathrm{d}\overrightarrow{L}_{\alpha,t}$$



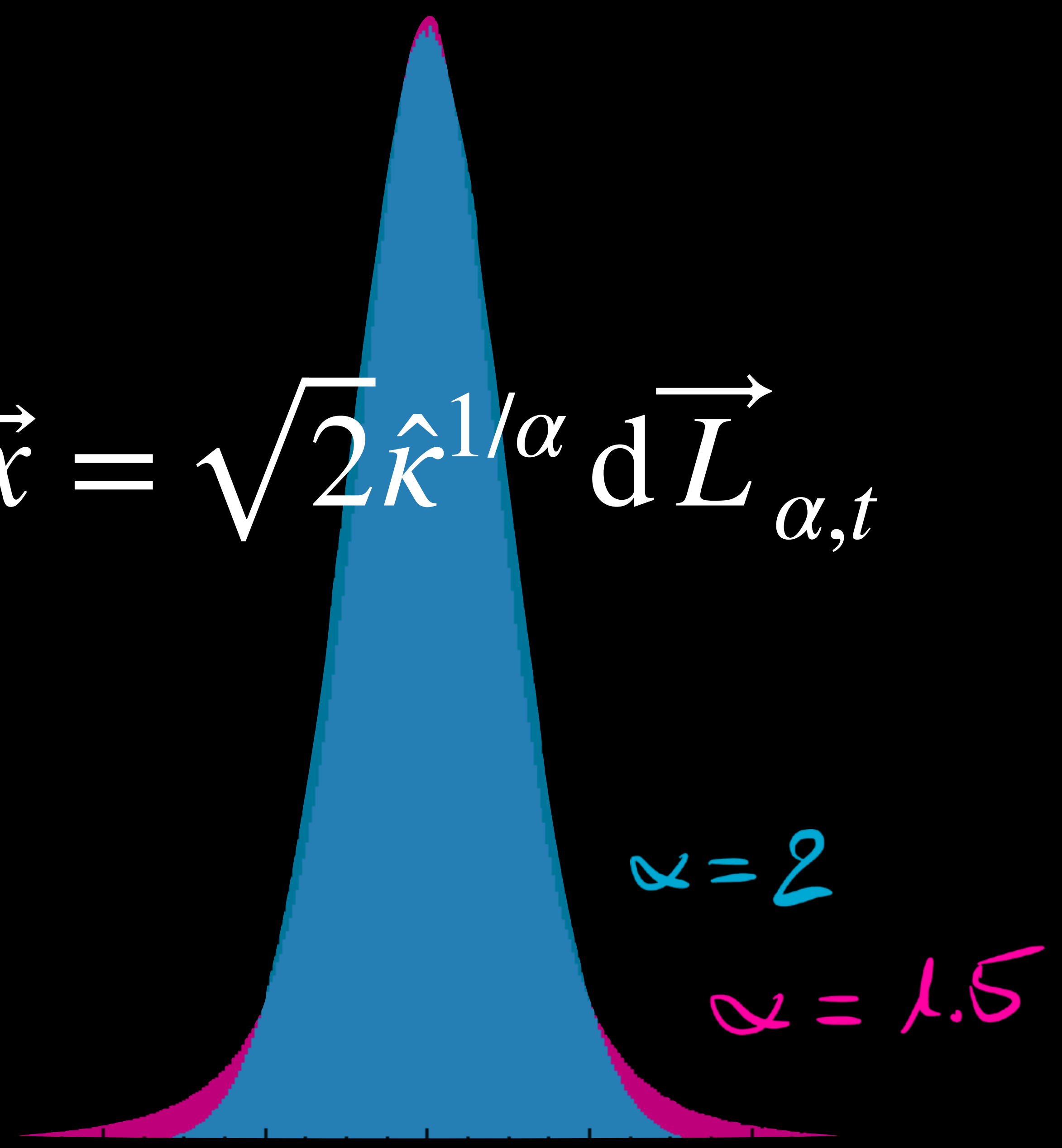
SUPERDIFFUSION

LEVY FLIGHTS





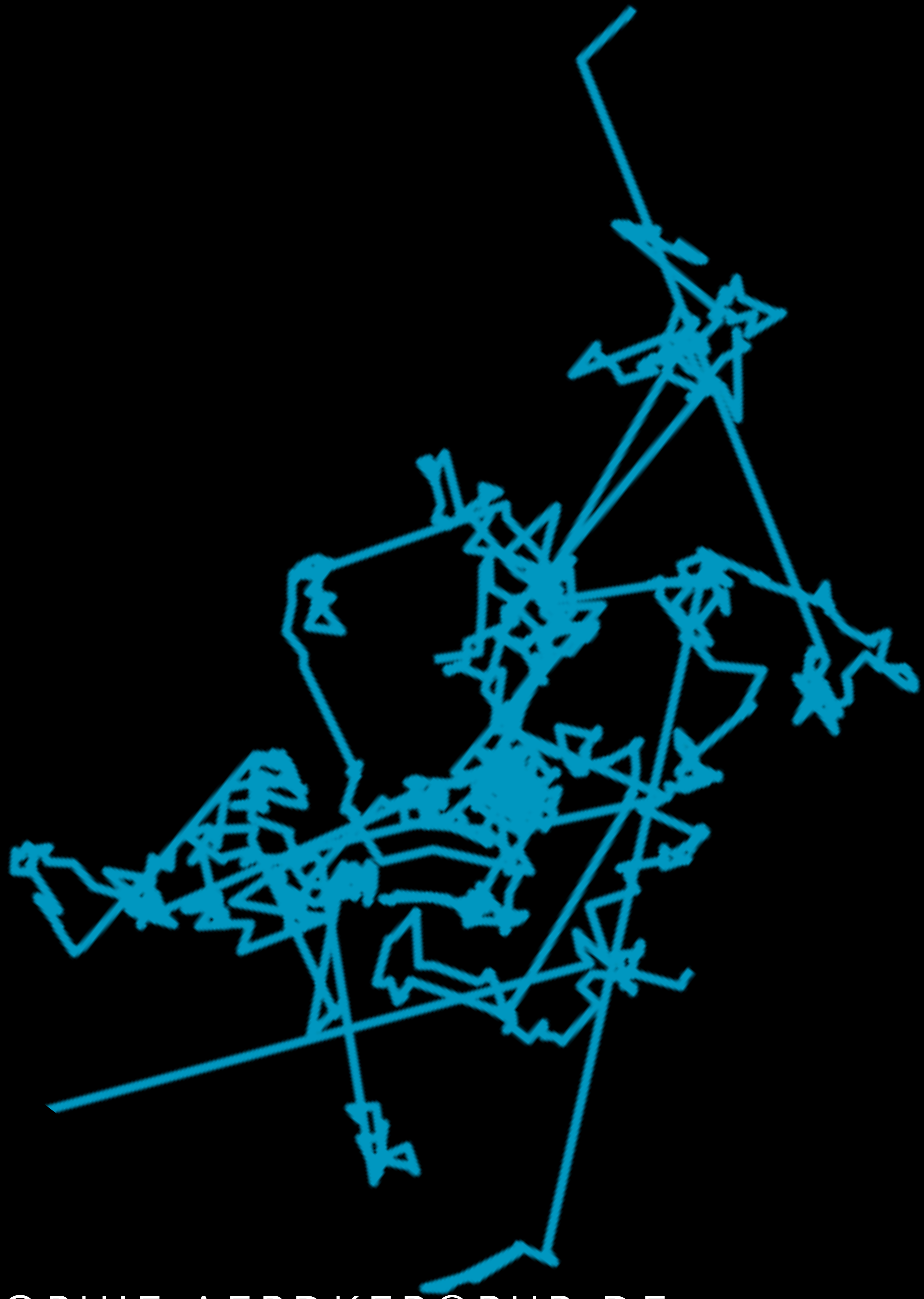
$$\mathrm{d}\vec{x} = \sqrt{2}\hat{\kappa}^{1/\alpha}\,\mathrm{d}\vec{L}_{\alpha,t}$$



TIME-DEPENDENT PARTICLE TRANSPORT

WITH STOCHASTIC DIFFERENTIAL EQUATIONS

- Fast & flexible approach:
  - Not dependent on source: Re-weighting and recycling of simulation data
  - Extension to anomalous diffusion
- Part of the CRPropa framework:
  - Magnetic field integration & magnetic field models
  - Interaction modules from CRPropa
- New application:
  - Stay tuned & reach out!



BACKUP

SUPERDIFFUSION

SOLVING FRACTIONAL TRANSPORT EQUATIONS

SFB1491 RUHR UNIVERSITÄT BOCHUM RUB

$$\langle (\Delta x)^2 \rangle \propto \kappa_\xi t^\xi$$

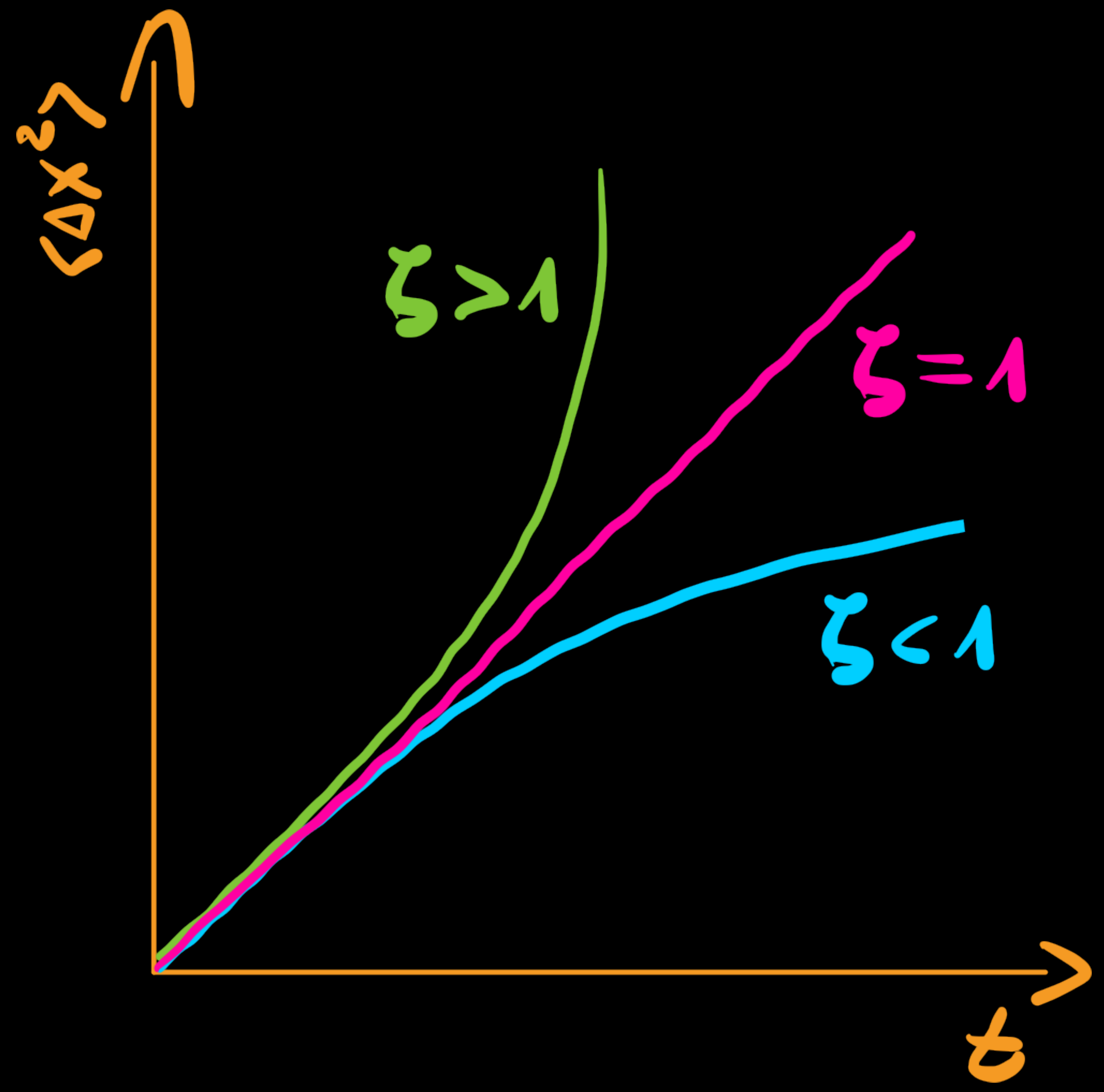
mean square displacement

generalized diffusion coefficient

$0 < \xi < 1$: subdiffusion

$\xi = 1$: normal (Gaussian) diffusion

$\xi > 1$: superdiffusion



SUPERDIFFUSION

SOLVING FRACTIONAL TRANSPORT EQUATIONS

$$\frac{\partial f(x,t)}{\partial t} = {}_0D_t^{1-\beta}\left(\frac{\partial}{\partial x}V'(x) + \kappa\nabla^{\alpha}\right)f(x,t)$$

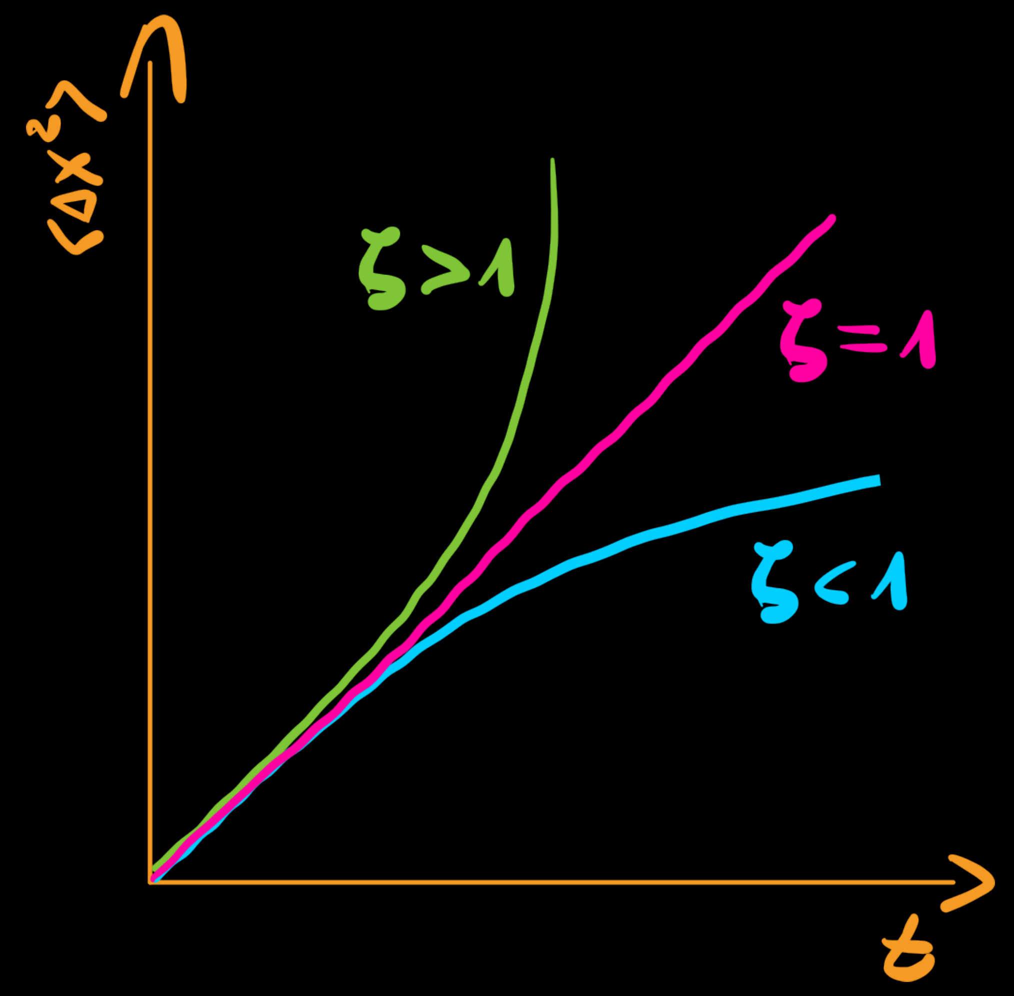
Riemann-Liouville fractional derivative

$= 1$ for $\beta = 1$

$\kappa = \kappa_\xi^{1/\xi}$

Riesz derivative

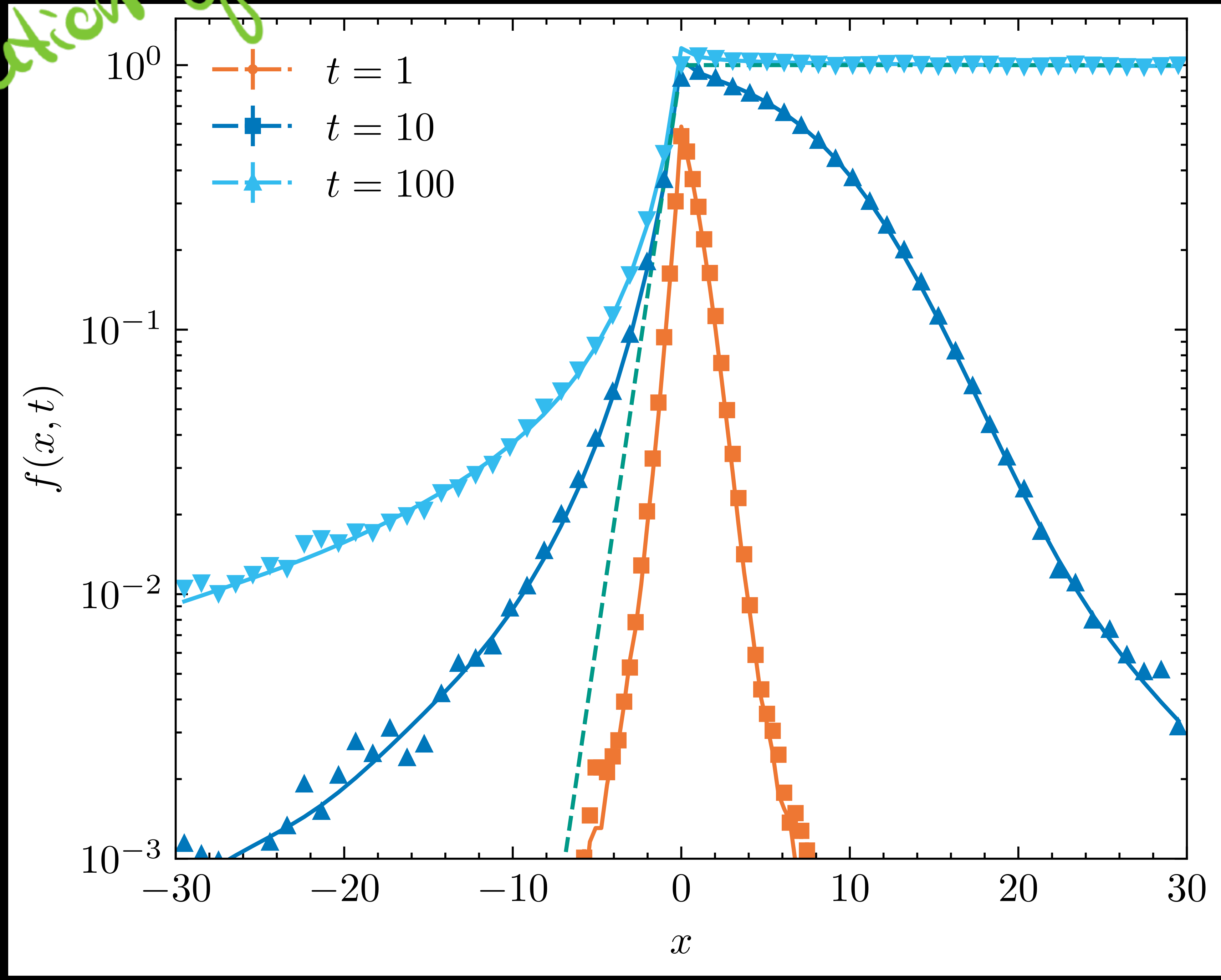
$= \nabla^2$ for $\alpha = 2$



SUPERDIFFUSIVE SHOCK ACCELERATION

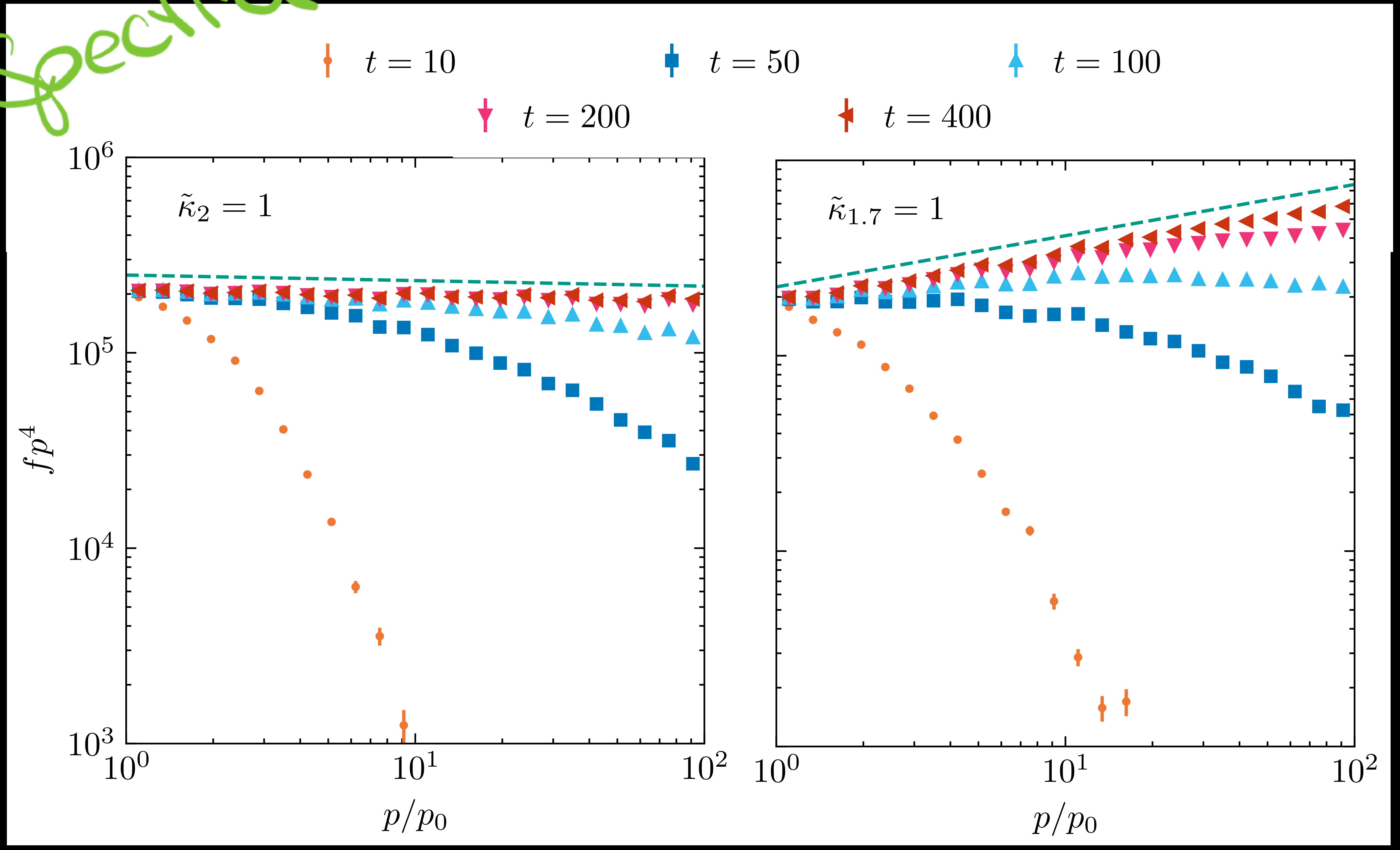
SFB1491 RUHR UNIVERSITÄT BOCHUM RUB

power-law distribution upstream



Effenberger, SA, et al., A&A (2024)

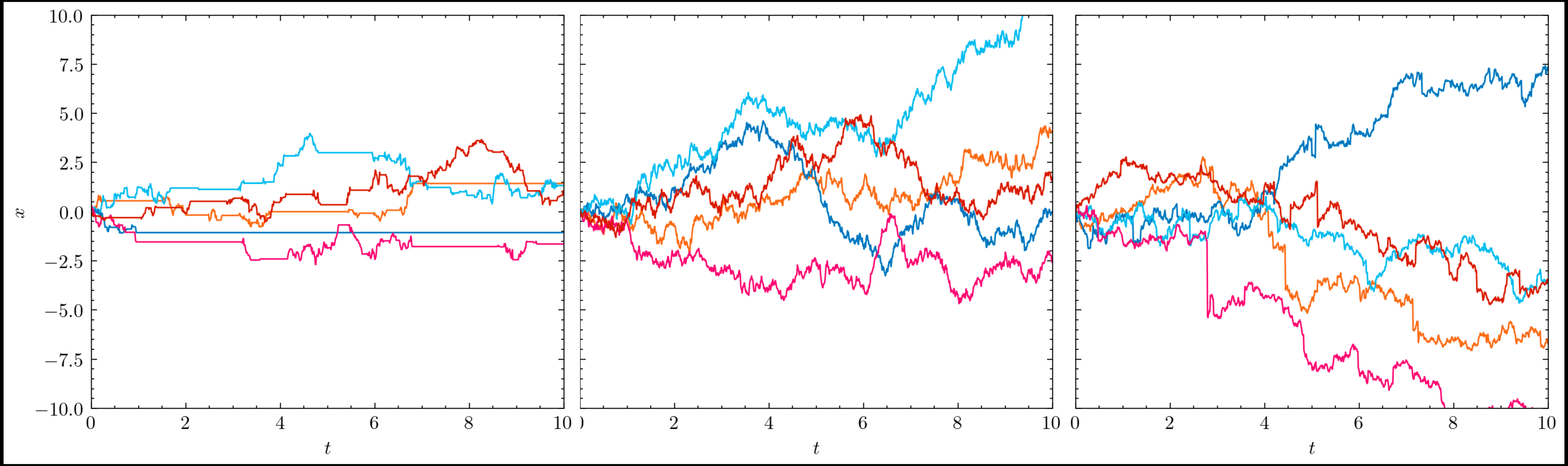
harder energy spectra



SA, et al., A&A (2025)

SUBDIFFUSION

INTRODUCING "WAITING TIMES"



Subdiffusion, "waiting times"
$< (\Delta x)^2 > \propto \kappa_\beta t^\beta$
Algorithm from Magdziarz, Weron 2007

Gaussian diffusion
$< (\Delta x)^2 > \propto \kappa t$
SDE with random numbers drawn from normal distribution

Superdiffusion, Lévy flights
$< (\Delta x)^2 > \propto \kappa_\alpha t^{2/\alpha}$
SDE with random numbers drawn from alpha-stable Lévy distribution

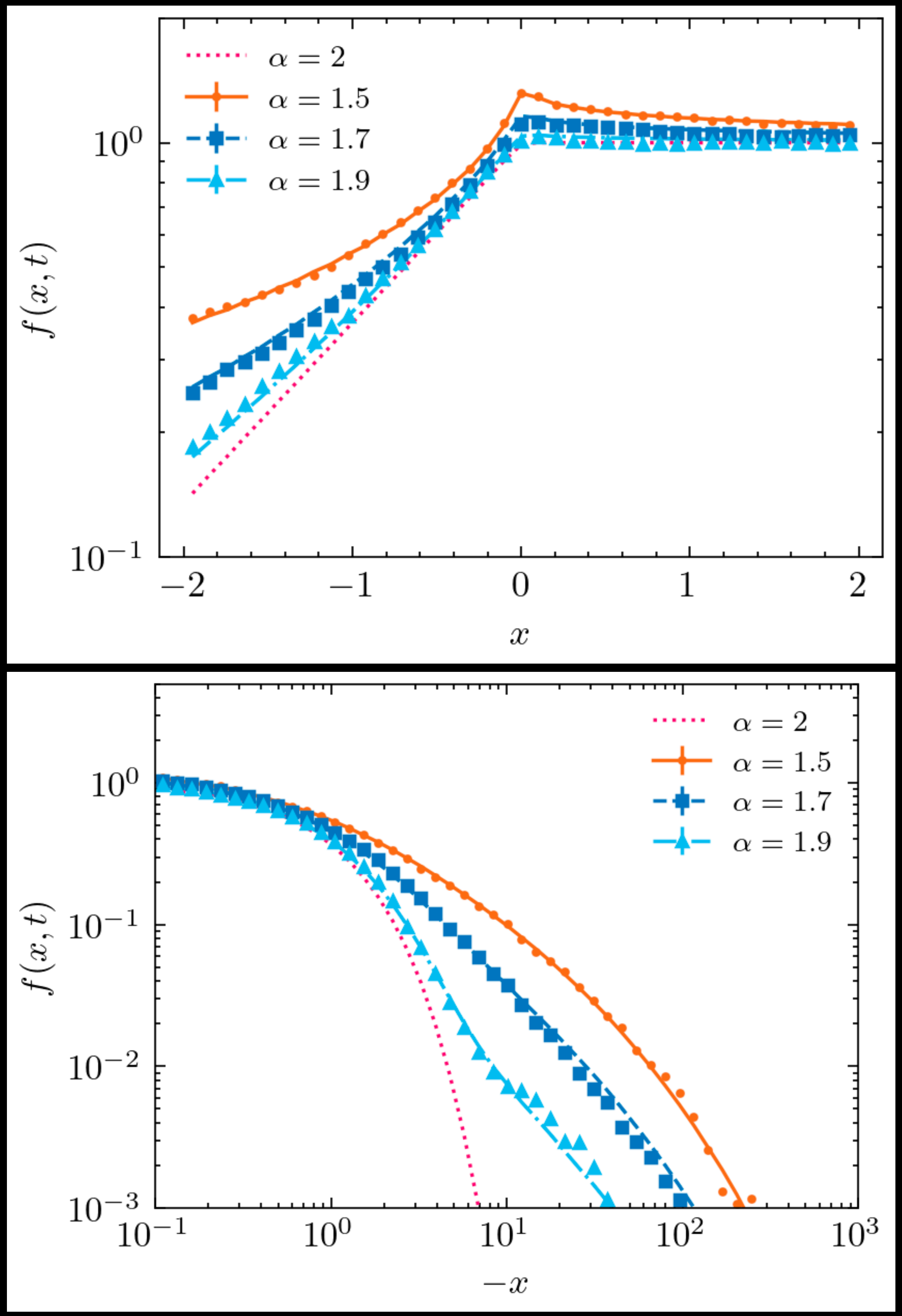
SUPERDIFFUSION

TRANSPORT AND ACCELERATION AT SHOCKS

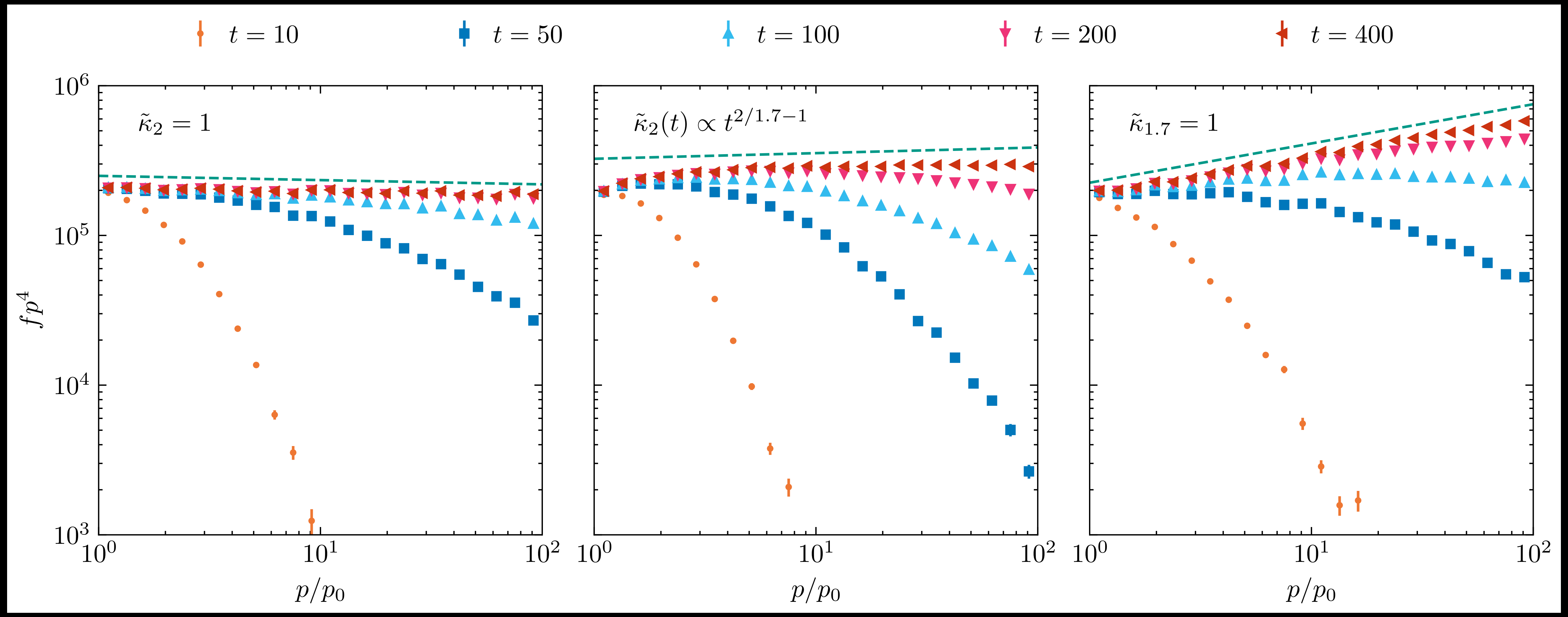
SFB1491

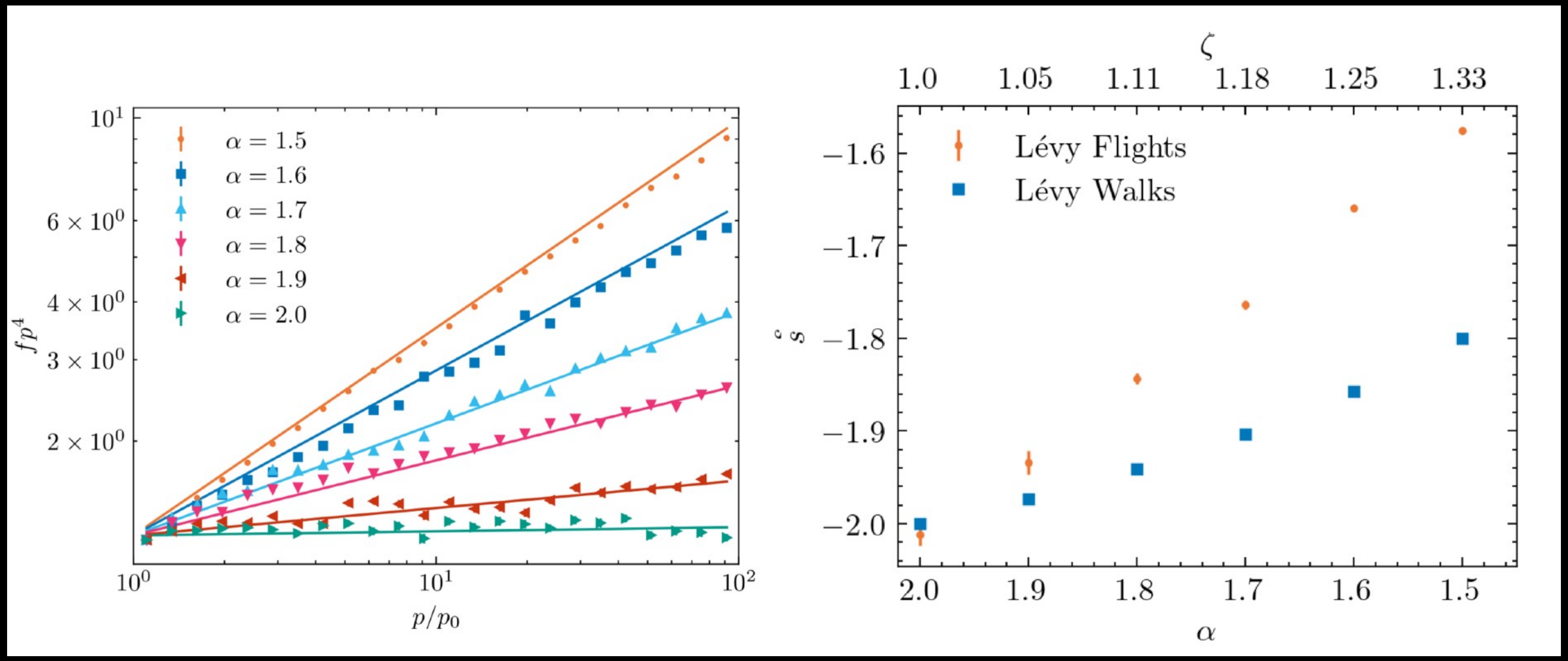
RUHR UNIVERSITÄT BOCHUM

RUB



Effenberger, SA, et al., A&A (2024)

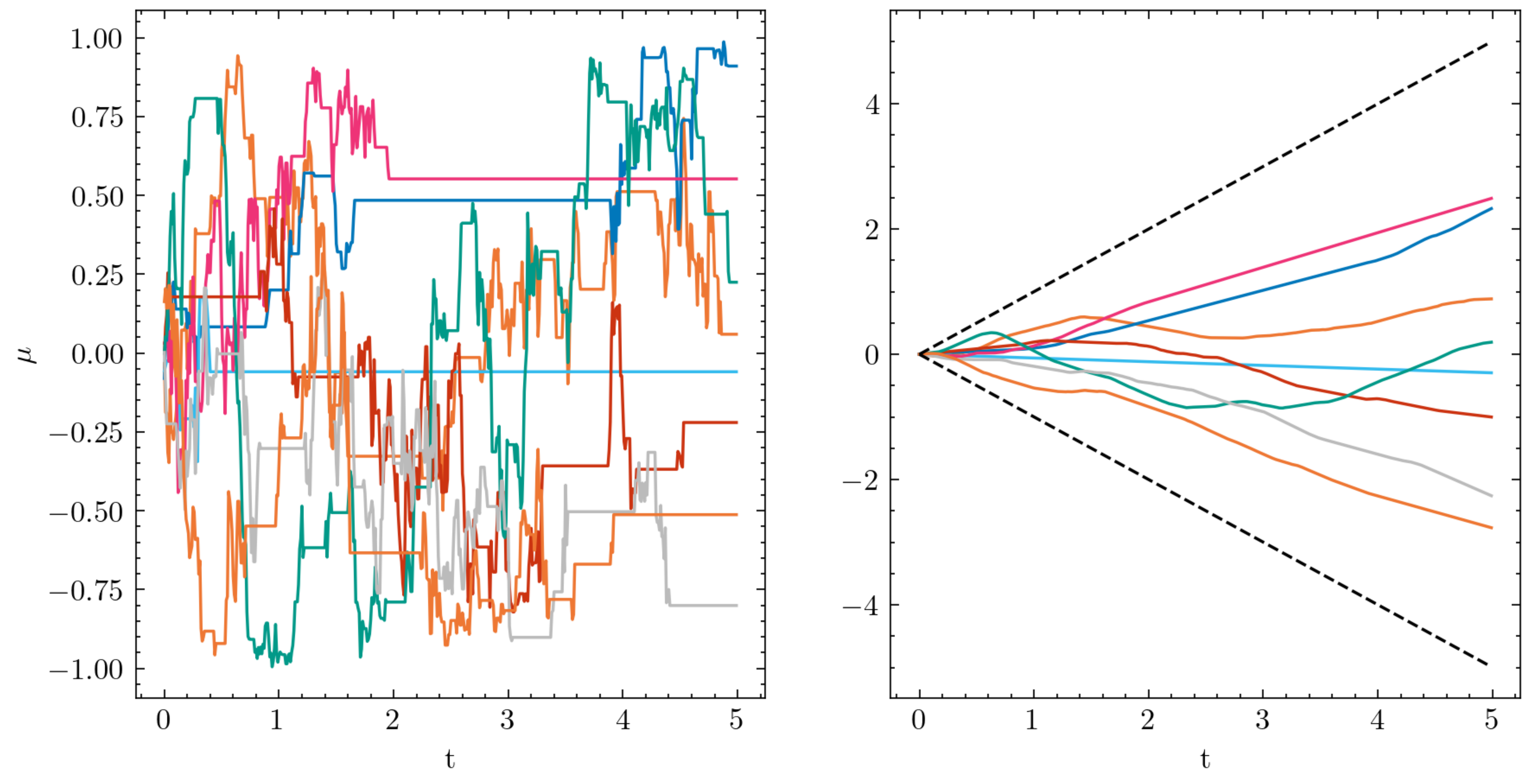




SA, et al., A&A (2025)

SUBDIFFUSION IN PITCH ANGLE

SUPERDIFFUSION IN SPACE



- Trapping in pitch-angle leads to superdiffusive behavior in space
- Bounded by the particle speed

CONTINUOUS INJECTION

APPROXIMATING STATIONARY STATES

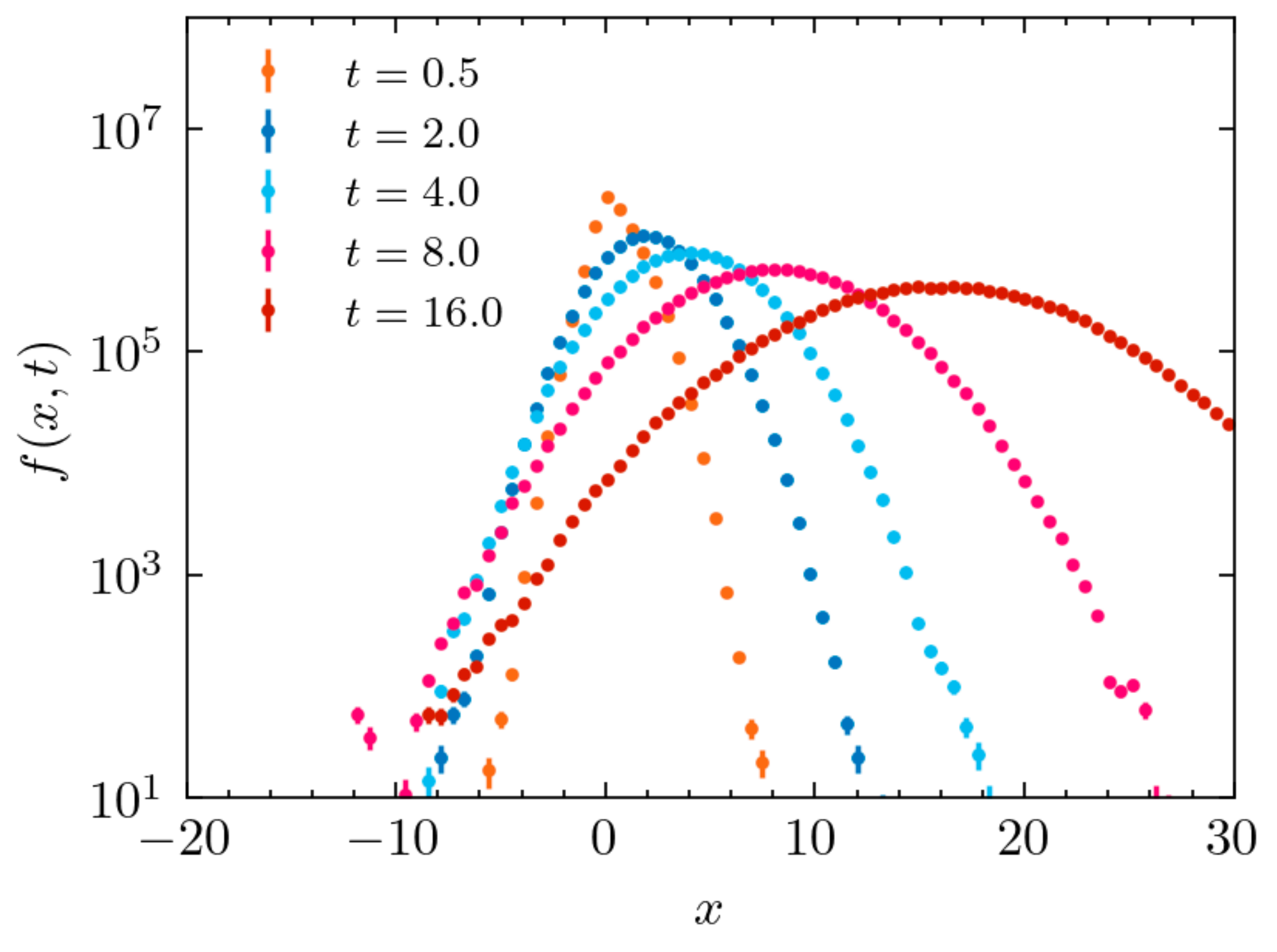
- Time integration approach: Superposition of the **Green's function** leads to general source term

➡ **Different sources** can be realized with a single simulation (by adjusting path amplitude)

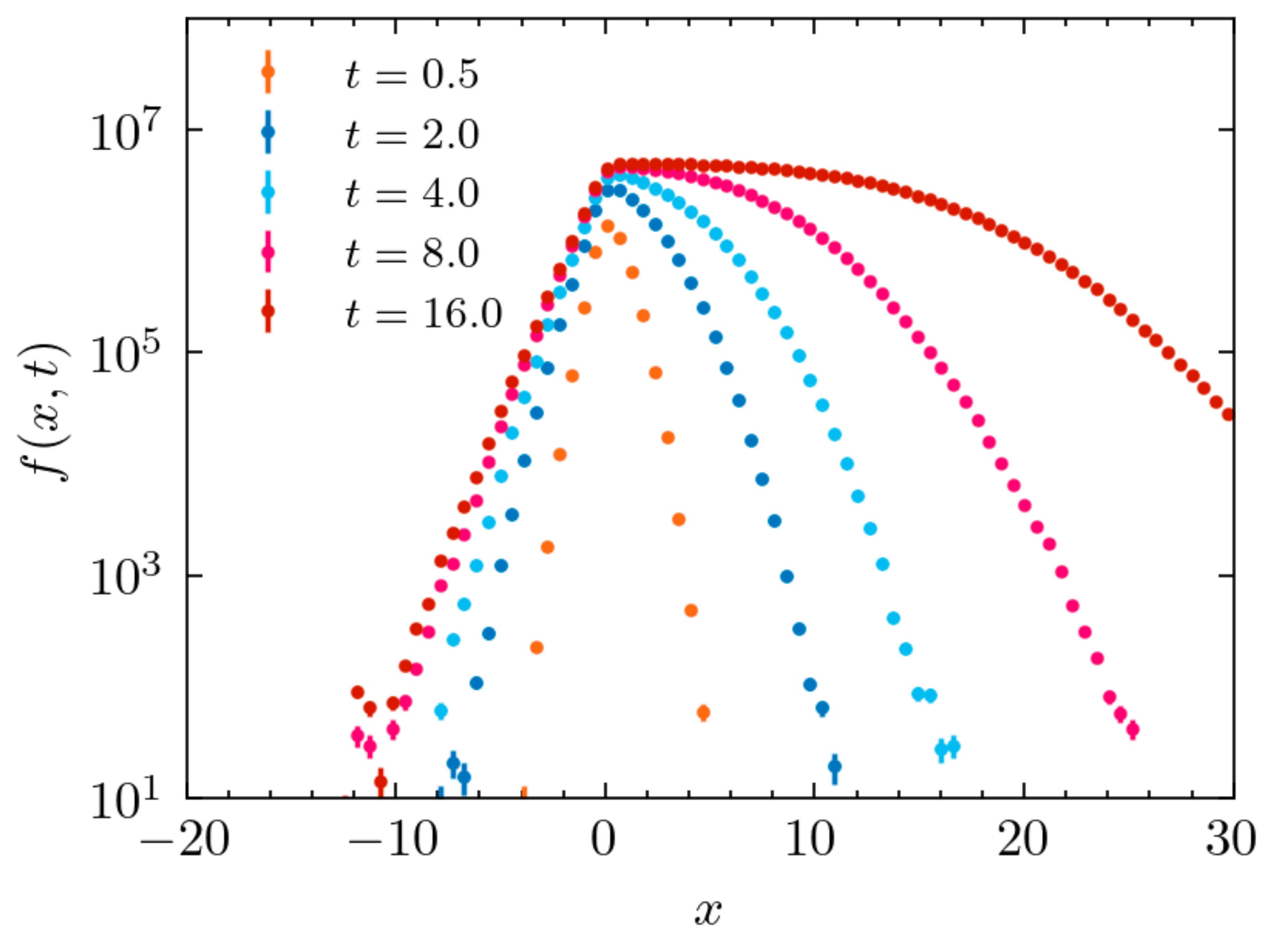
➡ The **resolution** of the time integration ΔT can be larger than the simulation time step Δt

- Works when solution **does not change much** during the time ΔT

Distribution $f_t(x)$ of pseudo-particles at time t with $S(x, t) = \delta(x)\delta(t)$



Summed distribution of pseudo-particles $f(x, t) = \sum_i f_t(x)\Delta T_i$ approximating the time integrated solution



TIME-DEPENDENT DSA

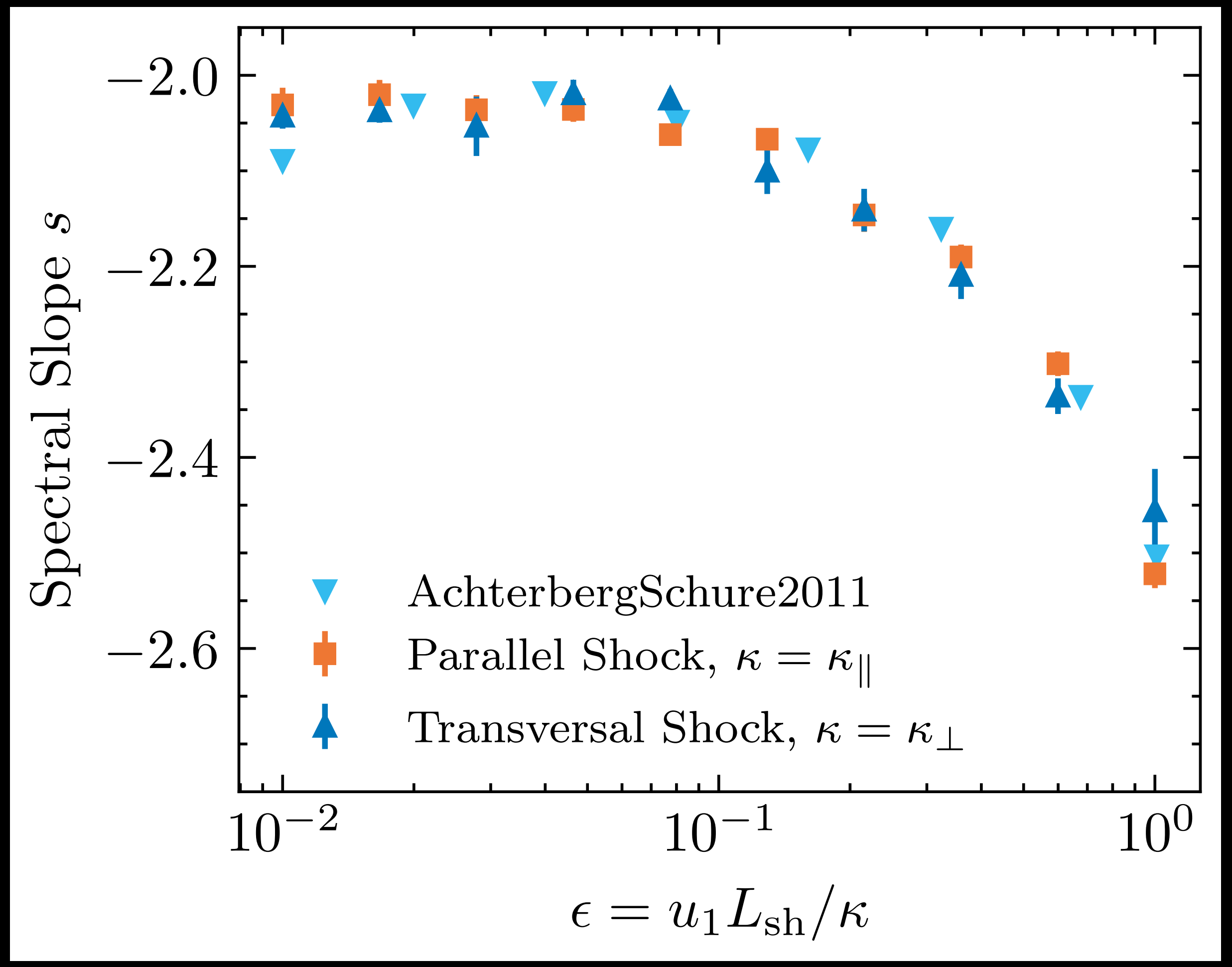
TIME STEP & SHOCK WIDTH

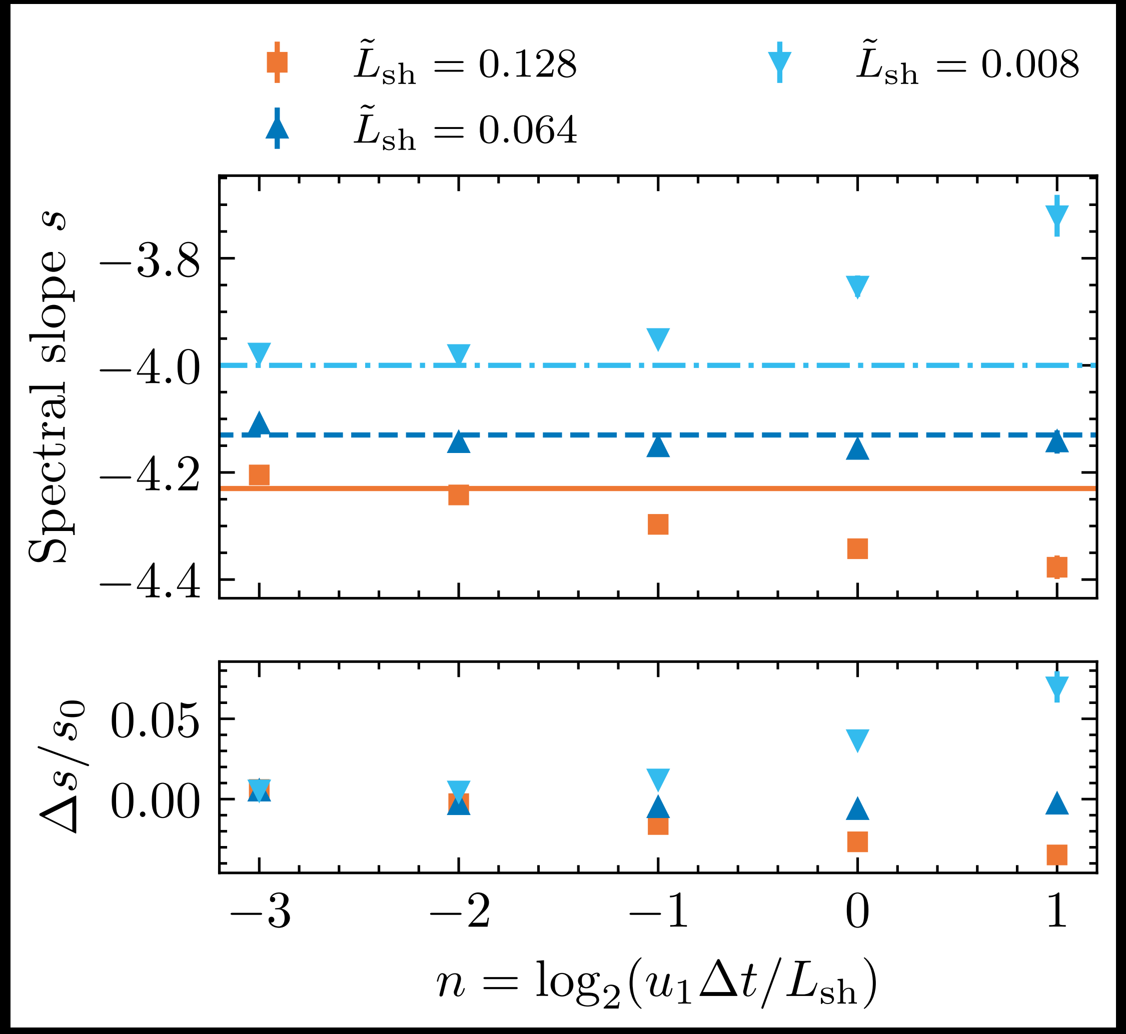
- Model shocks with **finite width** and different compression ratios

- **Adaptive step** that calculates the best time step for a given shock width according to

$$\left[\left(\nabla\cdot\hat{\kappa}\right)_{\parallel}+u_{\parallel}\right]\Delta t < L_{\mathrm{sh}} \lesssim \sqrt{2\kappa_{\parallel}\Delta t}$$

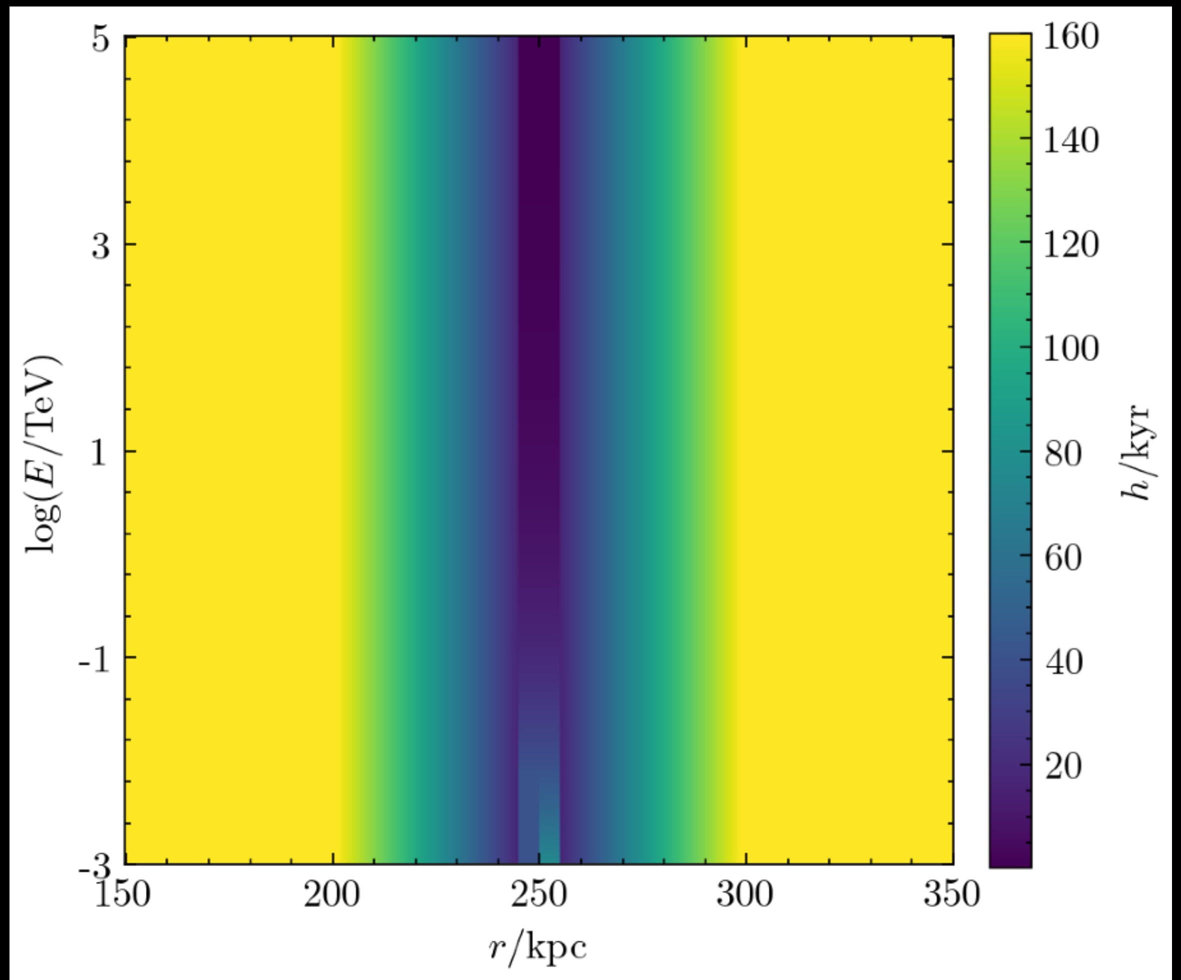
- Alternative: **Adaptive shockwidth** depending on energy





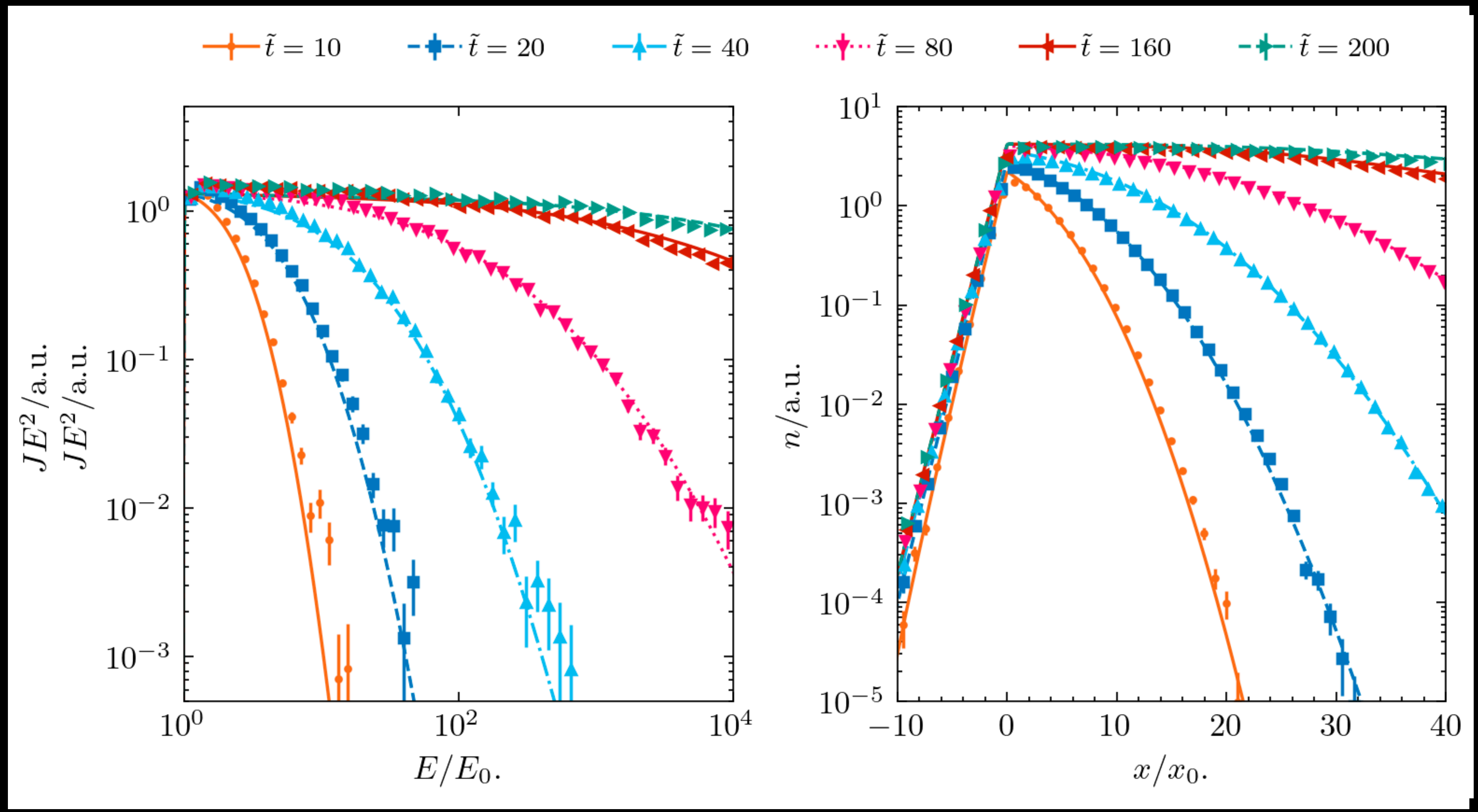
SA, et al., JCAP (2024)

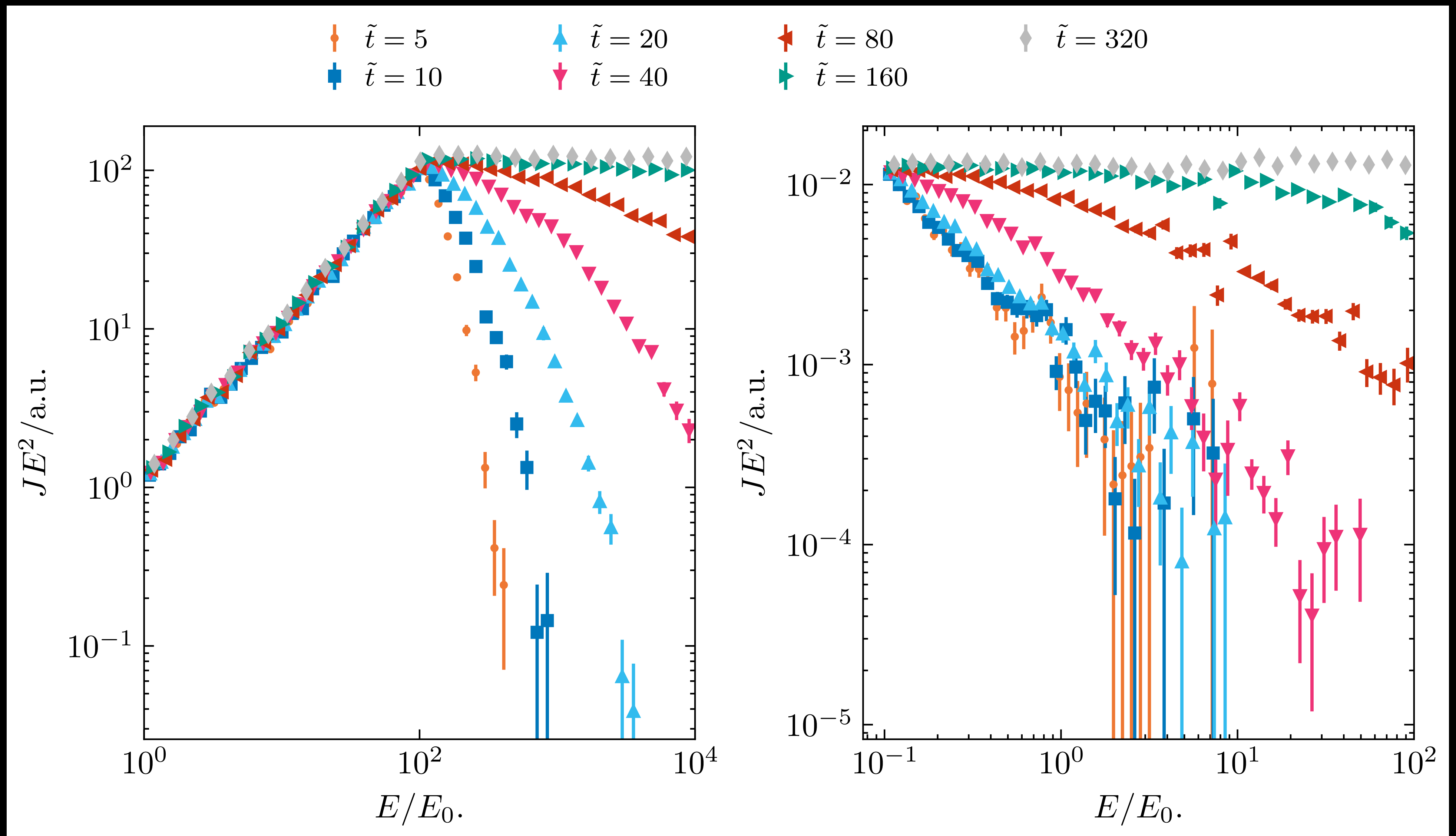
L. Merten & SA, CPC, 2025

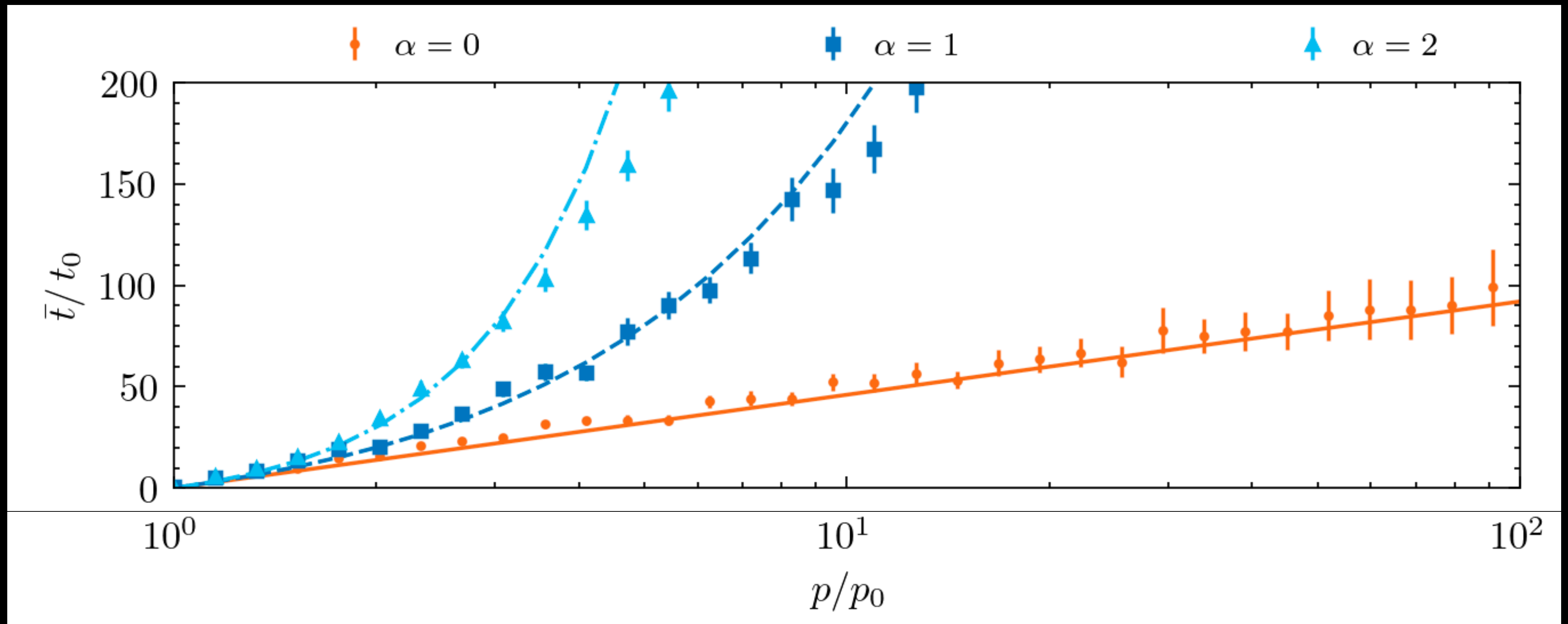


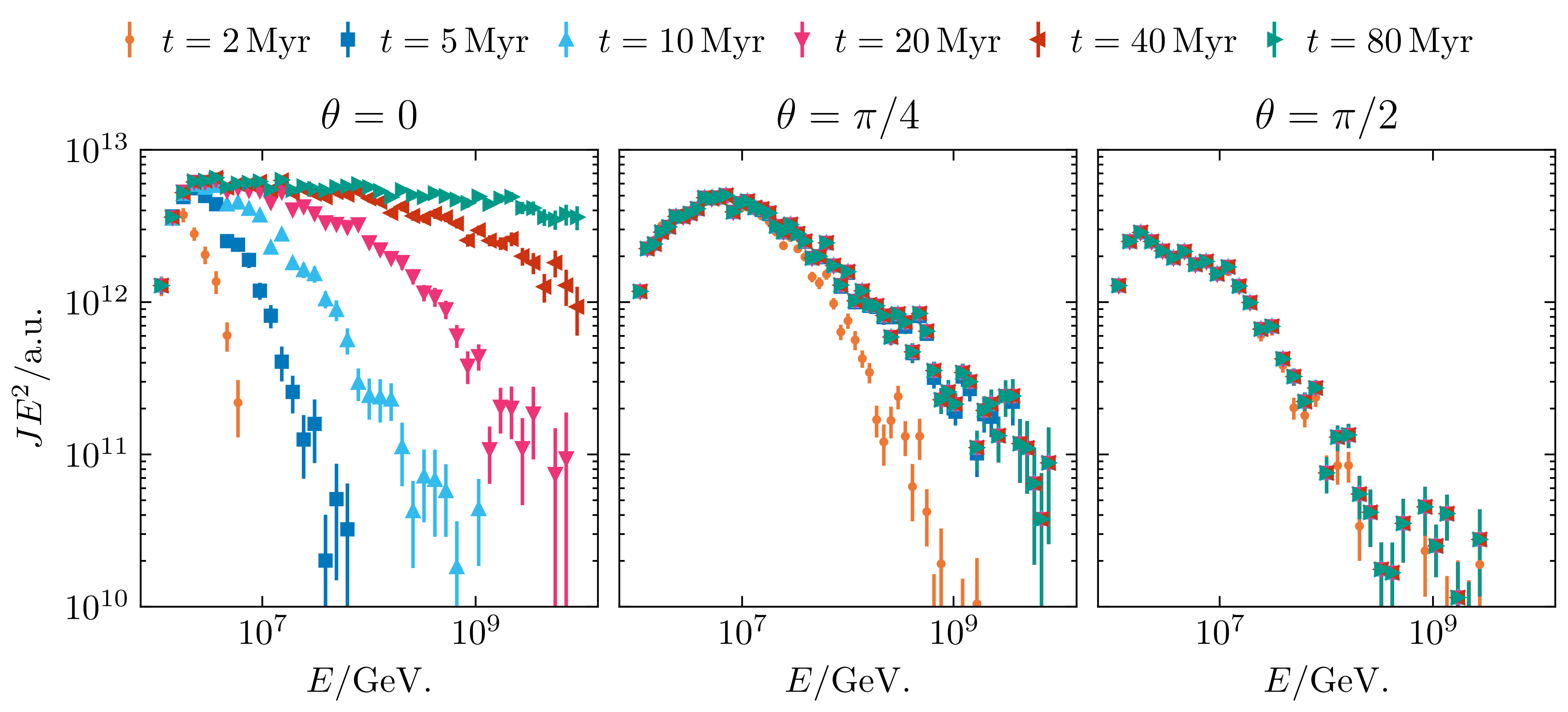
TIME-DEPENDENT DSA

FURTHER EXAMPLES





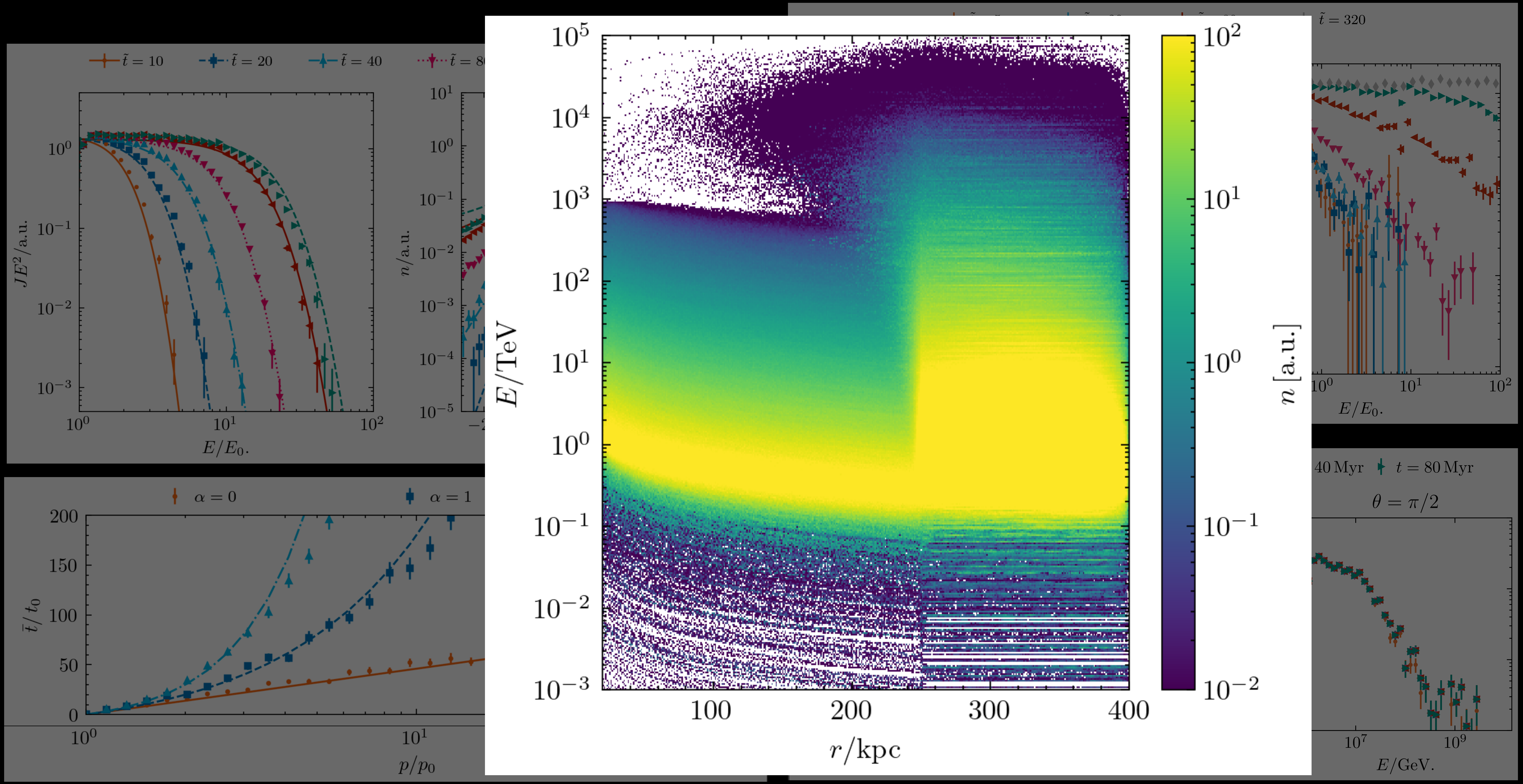




SA, et al., JCAP (2024)

TIME-DEPENDENT DSA

FURTHER EXAMPLES

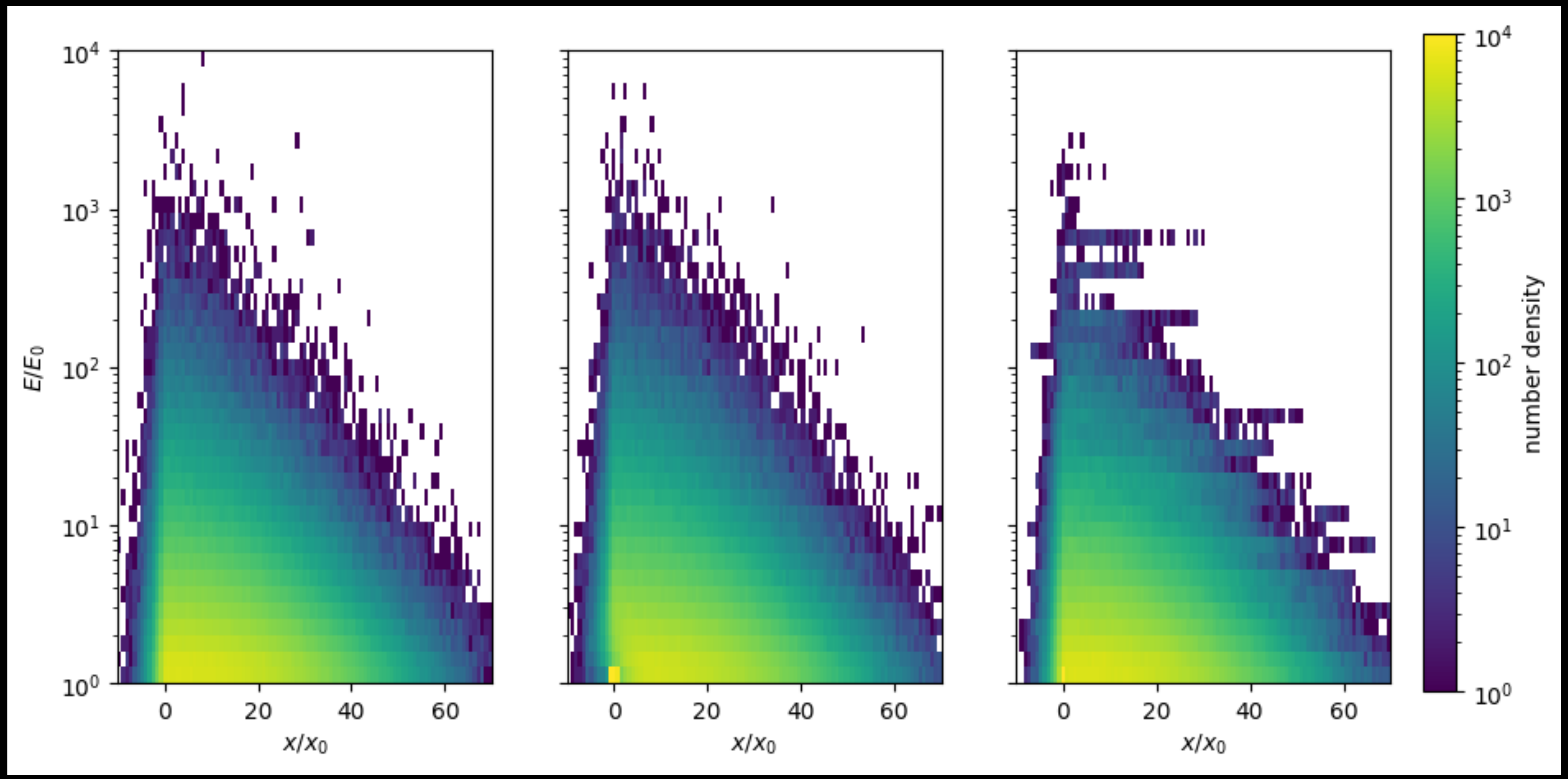


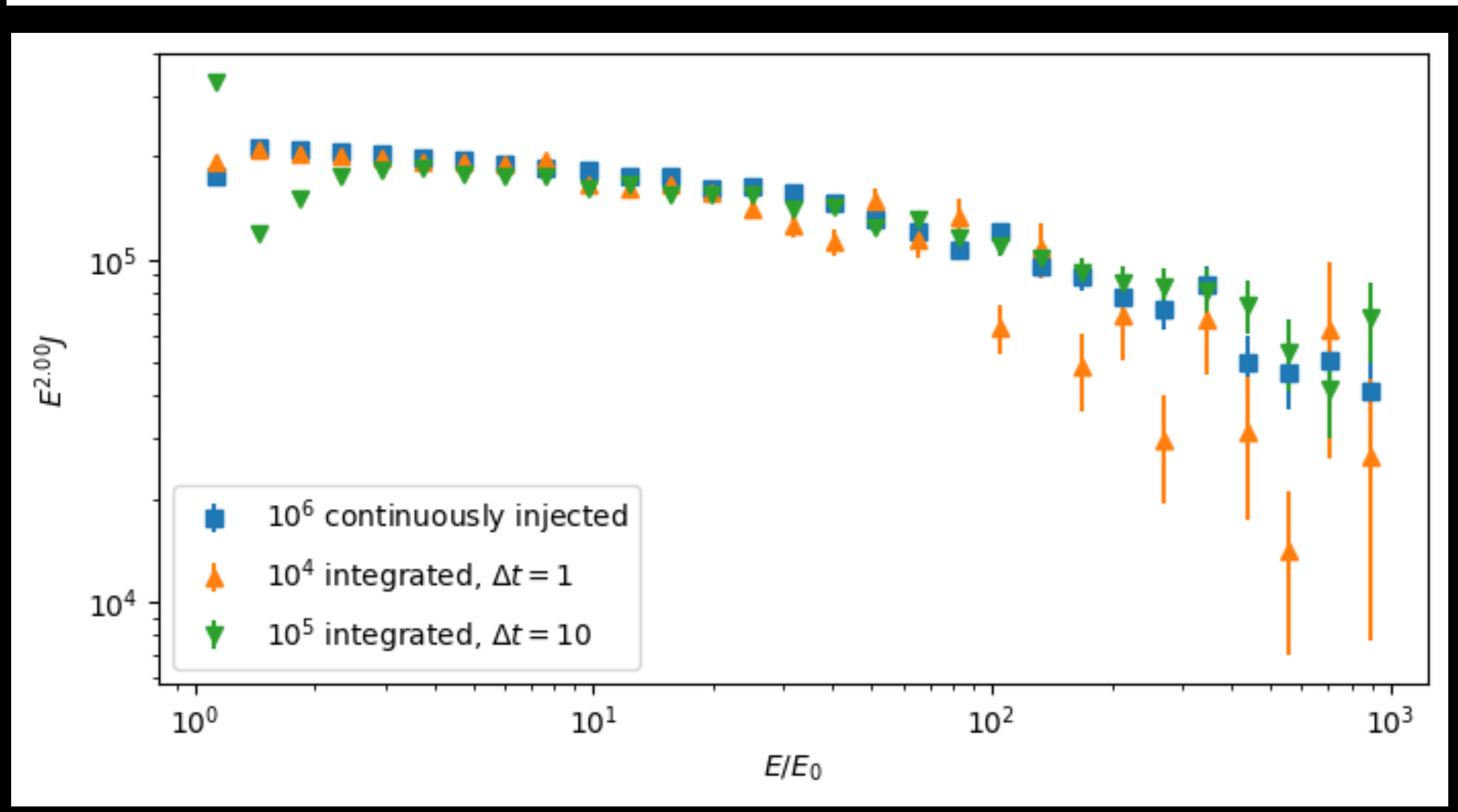
SA, et al., JCAP (2024)

UNCERTAINTIES

(IN)DEPENDENT PSEUDO-PARTICLES

- Underlying **Poisson noise**
- Pseudo-particles can **depend** on each other
  - ➡ Candidate splitting
  - ➡ Time integration
- Uncertainty due to **time integration** depends on
  - number of independent candidates
  - resolution in observing times ΔT



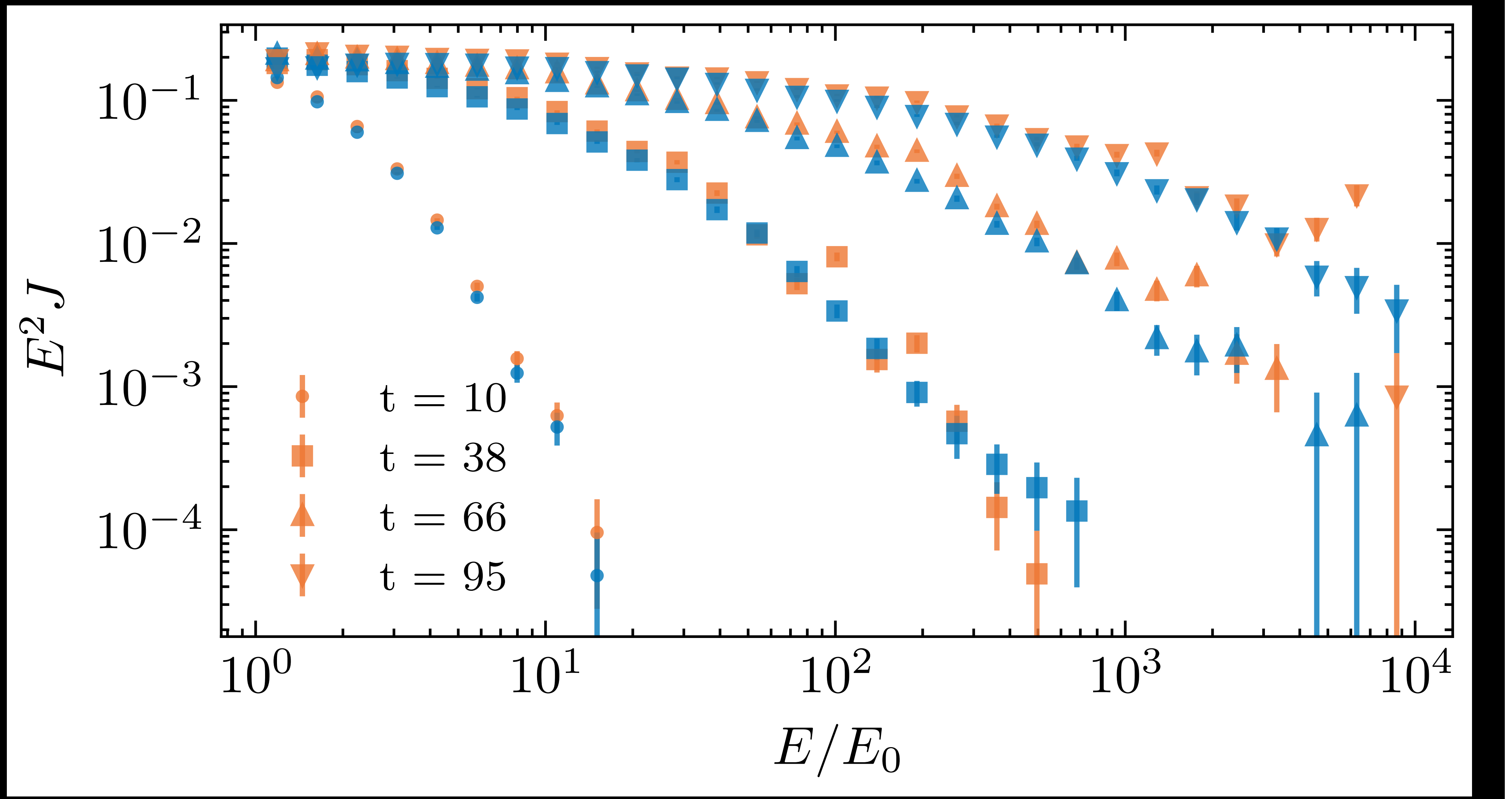


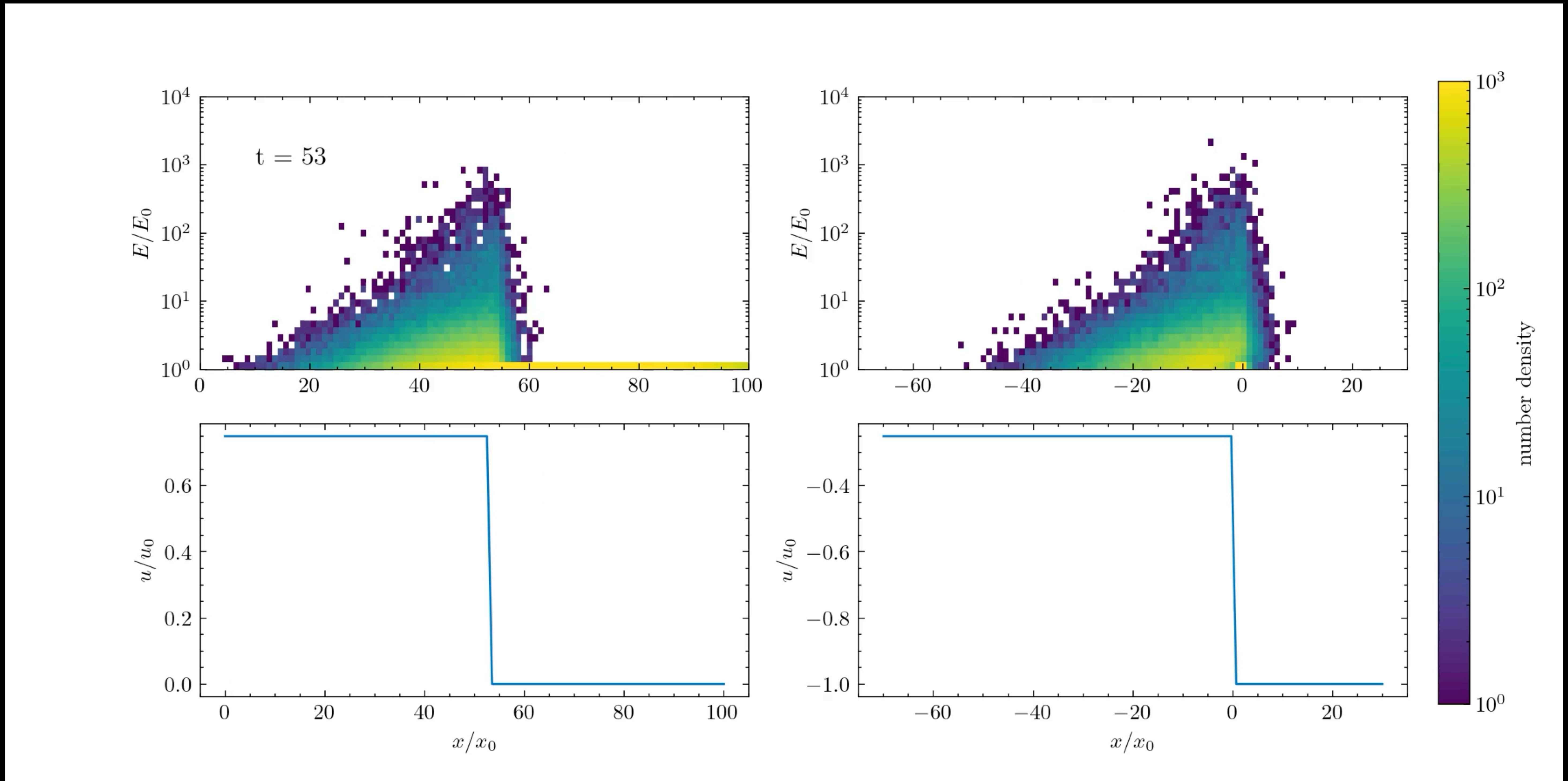
L. Merten & SA, CPC, 2025

MOVING SHOCKS

FROM STATIONARY TO LAB FRAME

Time evolution of energy spectra at the (moving) shock





SA, et al., arXiv:2501.14331

MOVING SHOCKS

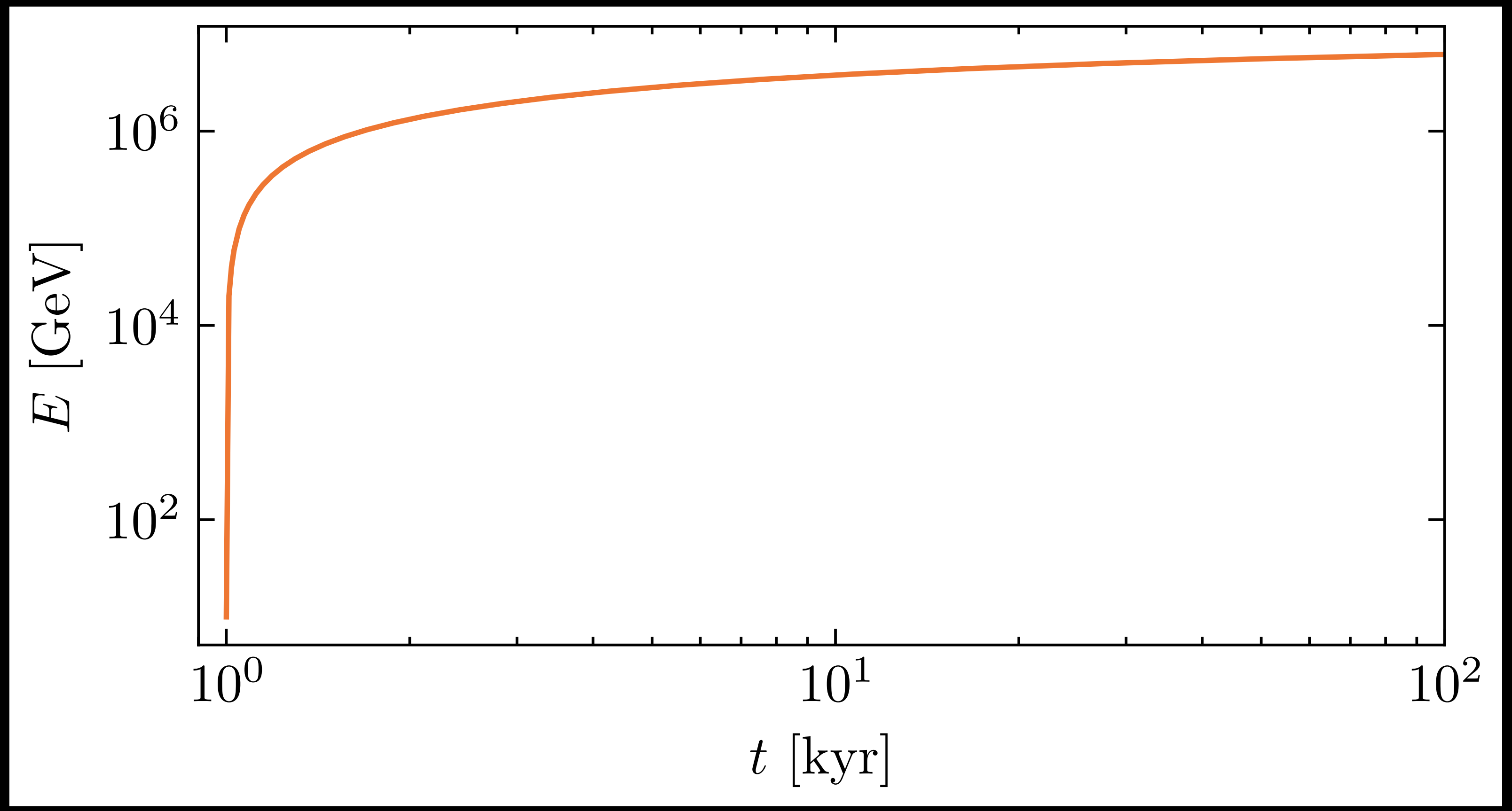
BLAST WAVES

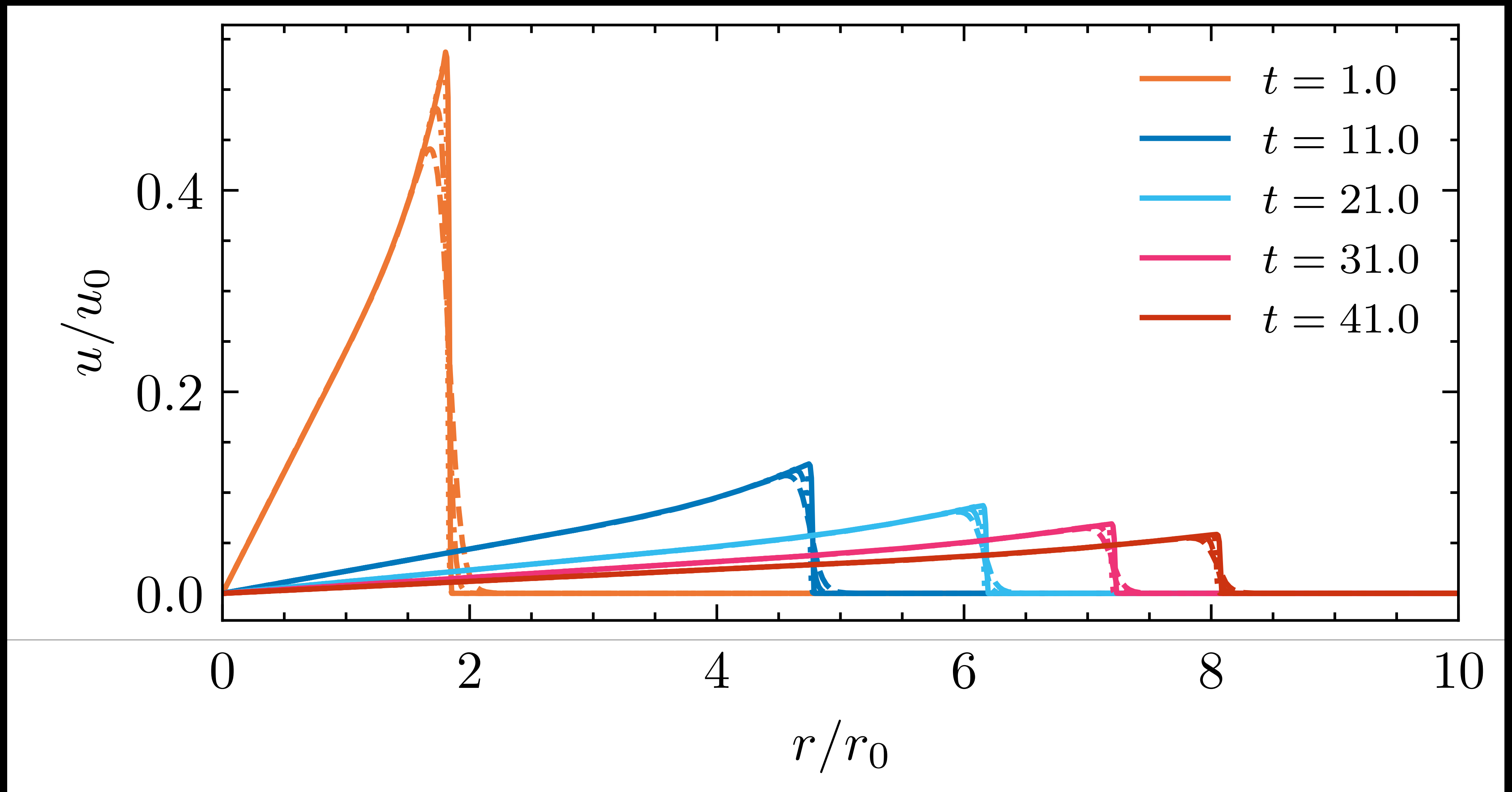
- Shock speed changes over time:

$$R(t) = \left(\frac{E_{\rm inj}}{\rho_0}\right)^{1/5} t^{2/5}$$

- **Adiabatic cooling** in the expanding wind behind the shock

- Fast acceleration early in time when the shock speed is high





SA, et al., arXiv:2501.14331

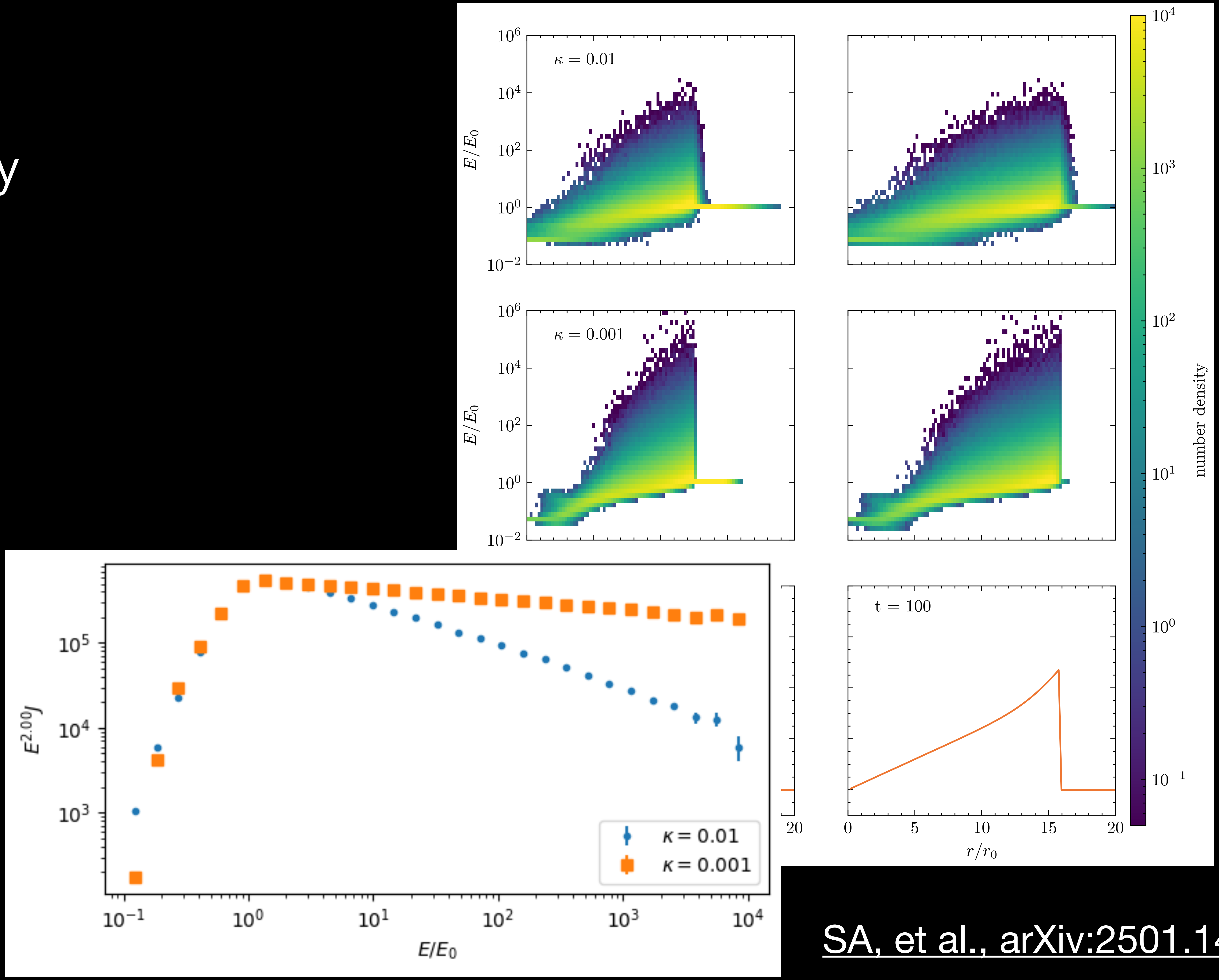
SPHERICAL BLAST WAVE

TIME-DEPENDENT EFFECTS

- Time-dependent advection $u(t, r)$ given by Sedov-Taylor similarity solution

- Corrections to the spectral slope $f \propto p^{-a}$ (Drury, 1983)

$$a = 4\left[1 + (3+b)\left(\frac{\kappa_1}{Ru_1} + \frac{\kappa_2}{Ru_2}\right) + \frac{\kappa_2}{Ru_2}\right] + O(\epsilon^2)$$



SA, et al., arXiv:2501.14331