PRECISE summer school
Warsaw

July 03, 2023

hands-on cosmological simulations

session 1: background and the N-body method

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&
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Durham University

lecture notes:
https://github.com/sownakbose/PRECISE_Summer_School_Sims

jupyter notebooks:
https://github.com/Shaun-T-Brown/Summer_school

objectives of this course

- give you some historical context of cosmological simulations and how they aid us understand the universe
- a (brief) introduction to some of the numerical techniques used in modern codes
- how to set up initial conditions and introduce cosmology to an N-body simulations
- algorithms for identifying nonlinear structures (haloes and subhaloes) in a particle distribution
- figure out how to design and run your own simulations
- learn techniques for analysing the outputs of simulations
- appreciate where simulations are useful, but also what their limitations are!

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structures are coupled across multiple scales

large-scale structure
[~ 10^9 light-years]

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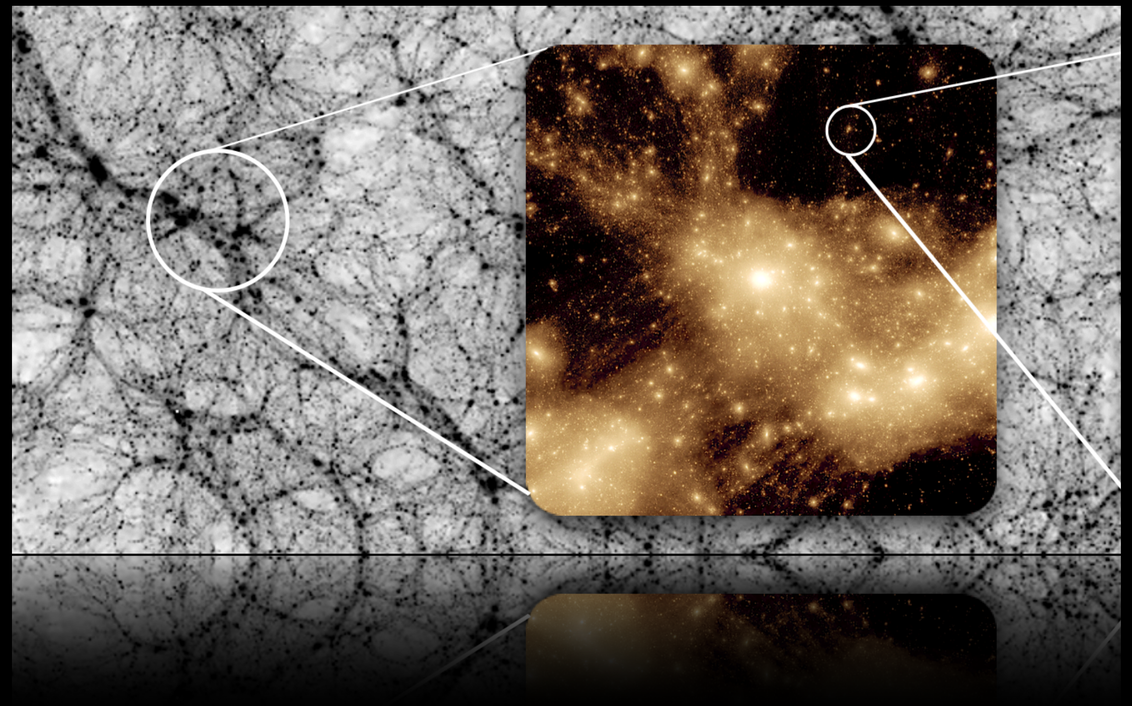
dark matter haloes
[~ 10^6 light-years]



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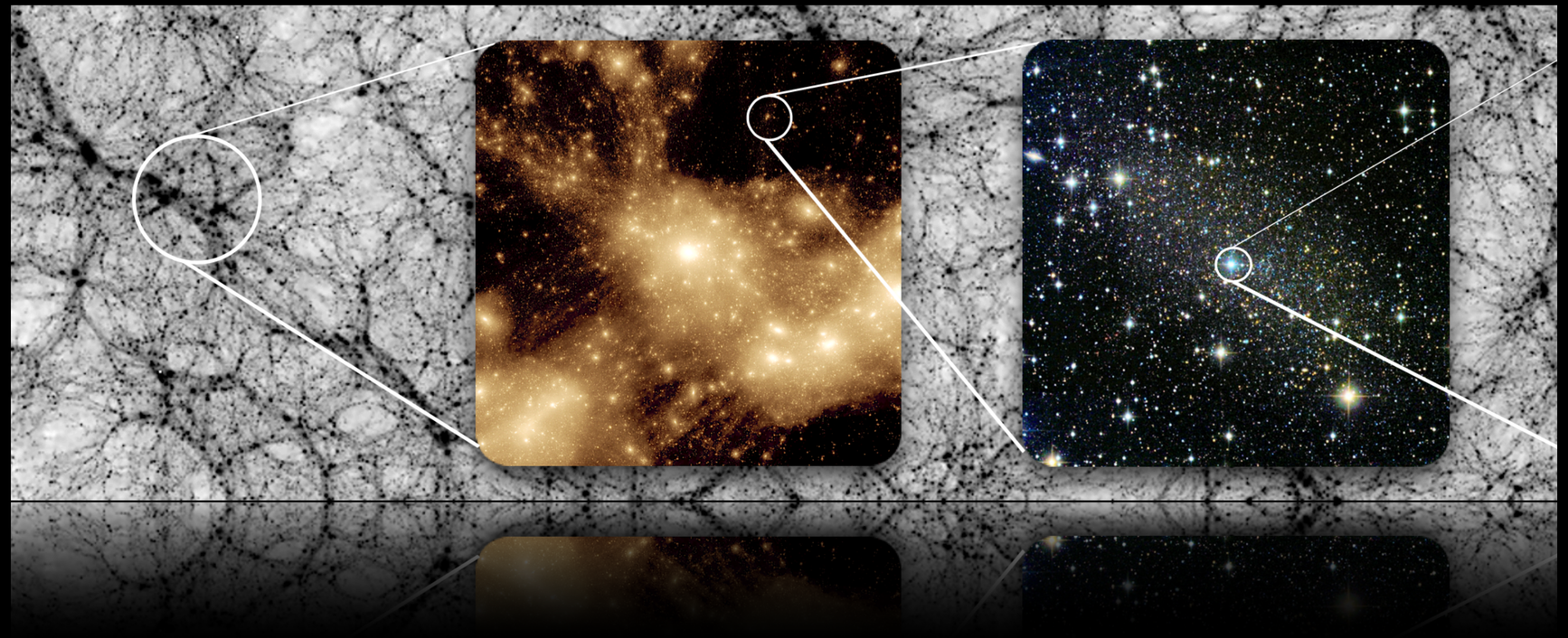

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dark matter haloes
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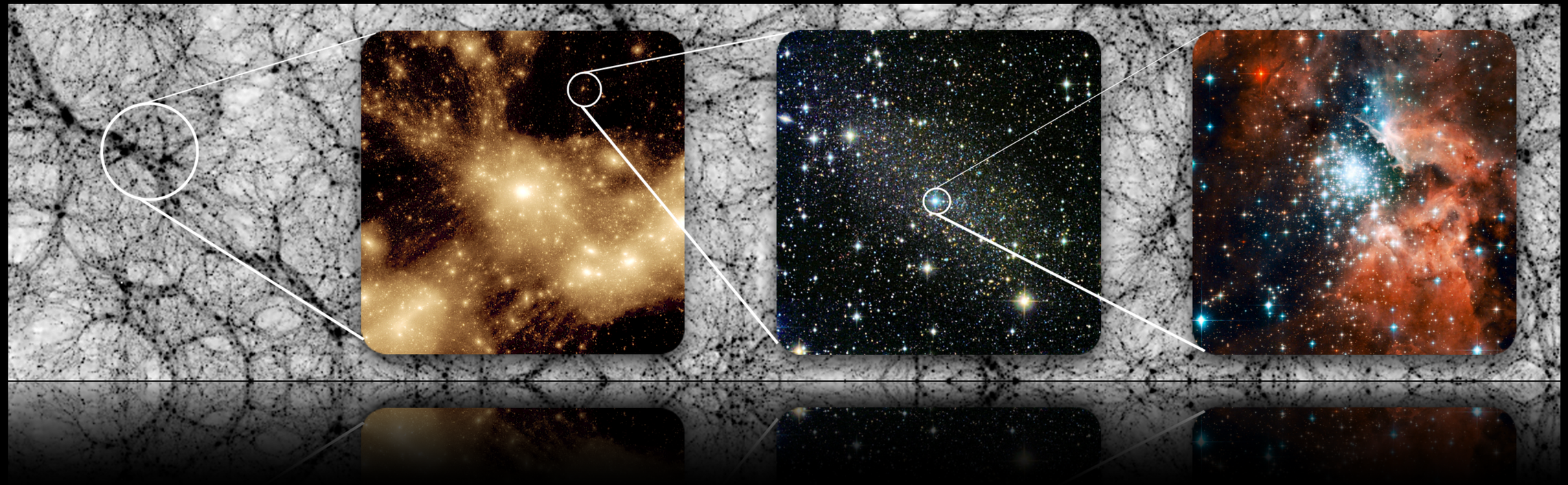
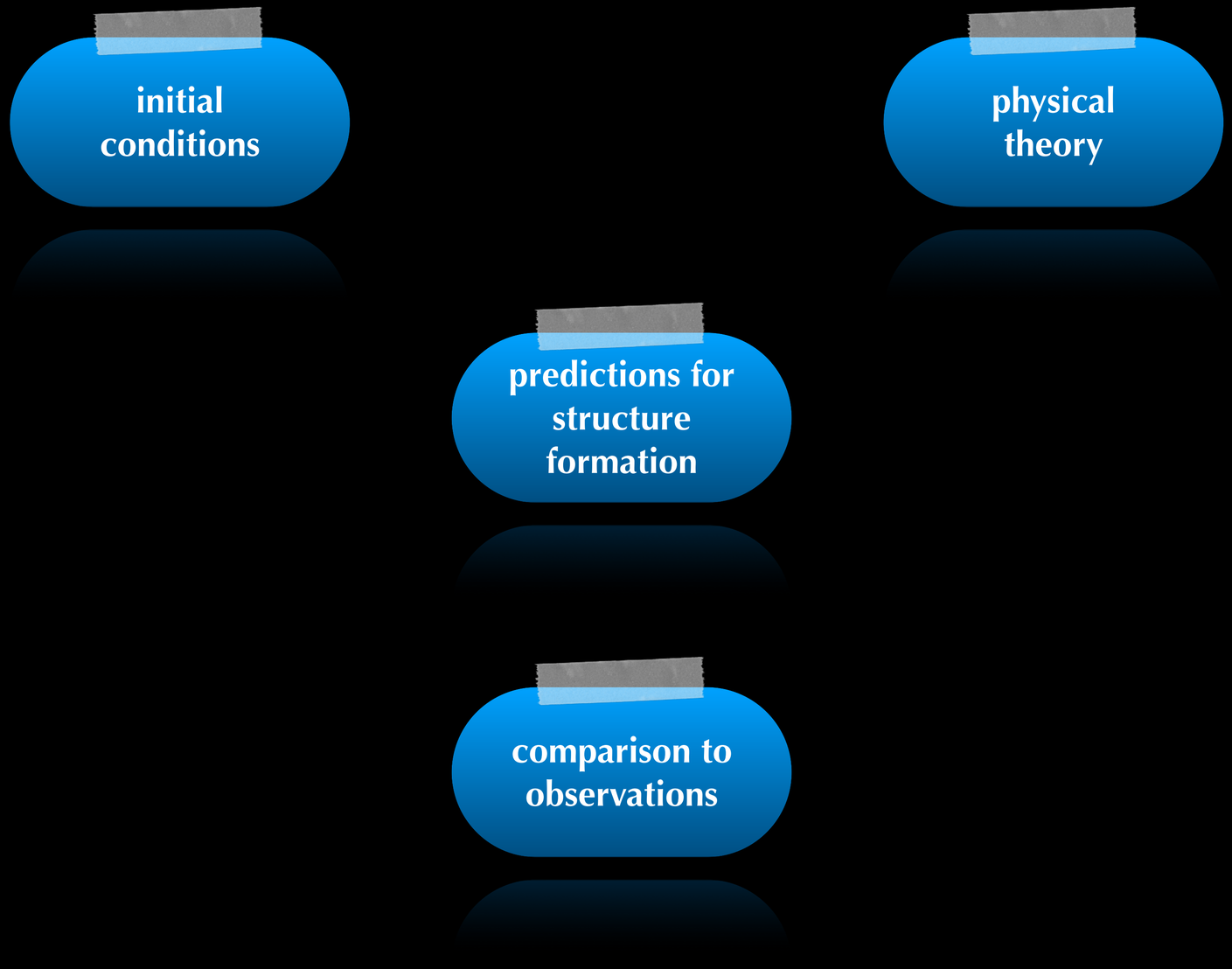
star formation sites
[~ light-years]



the pathway to simulating the cosmos



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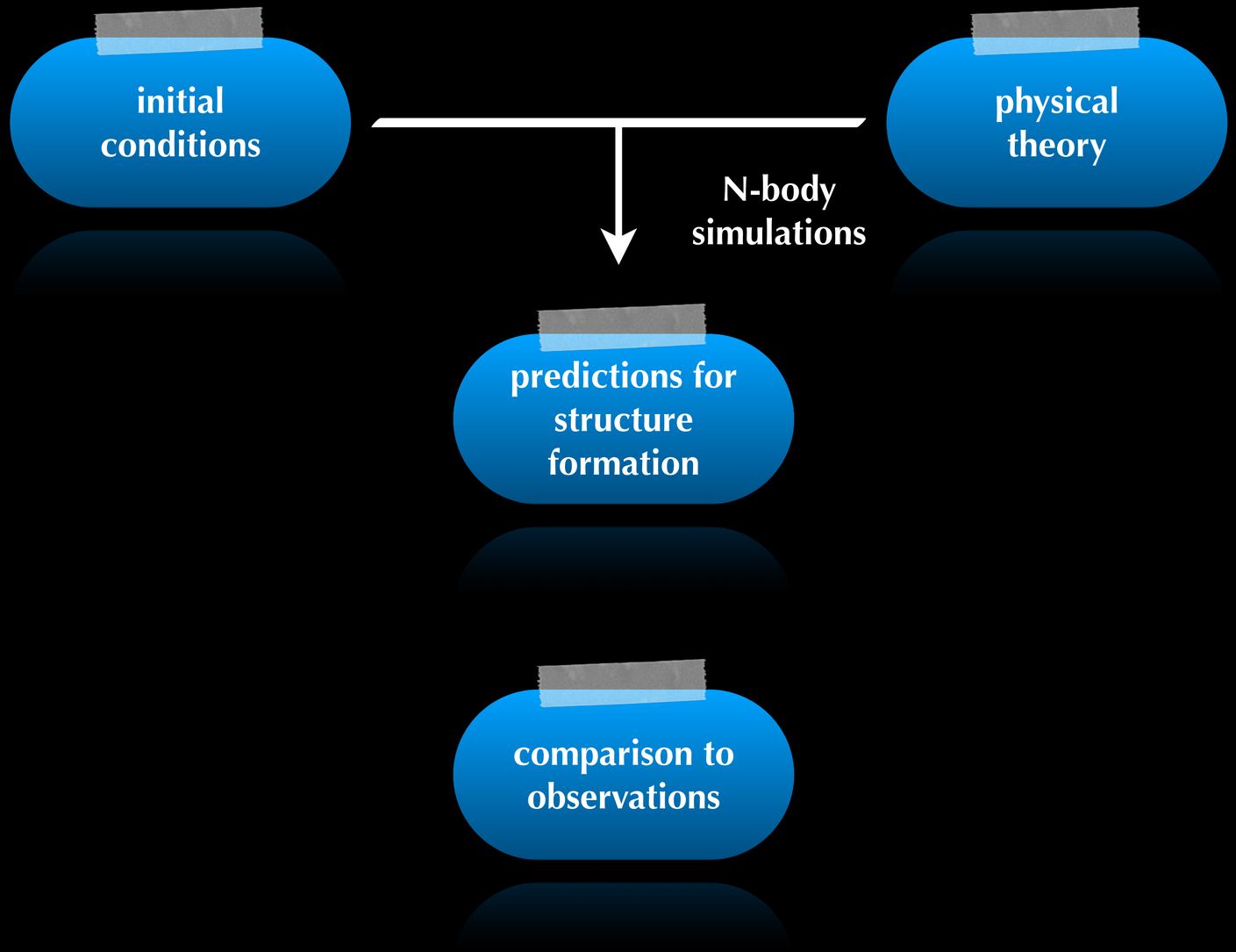

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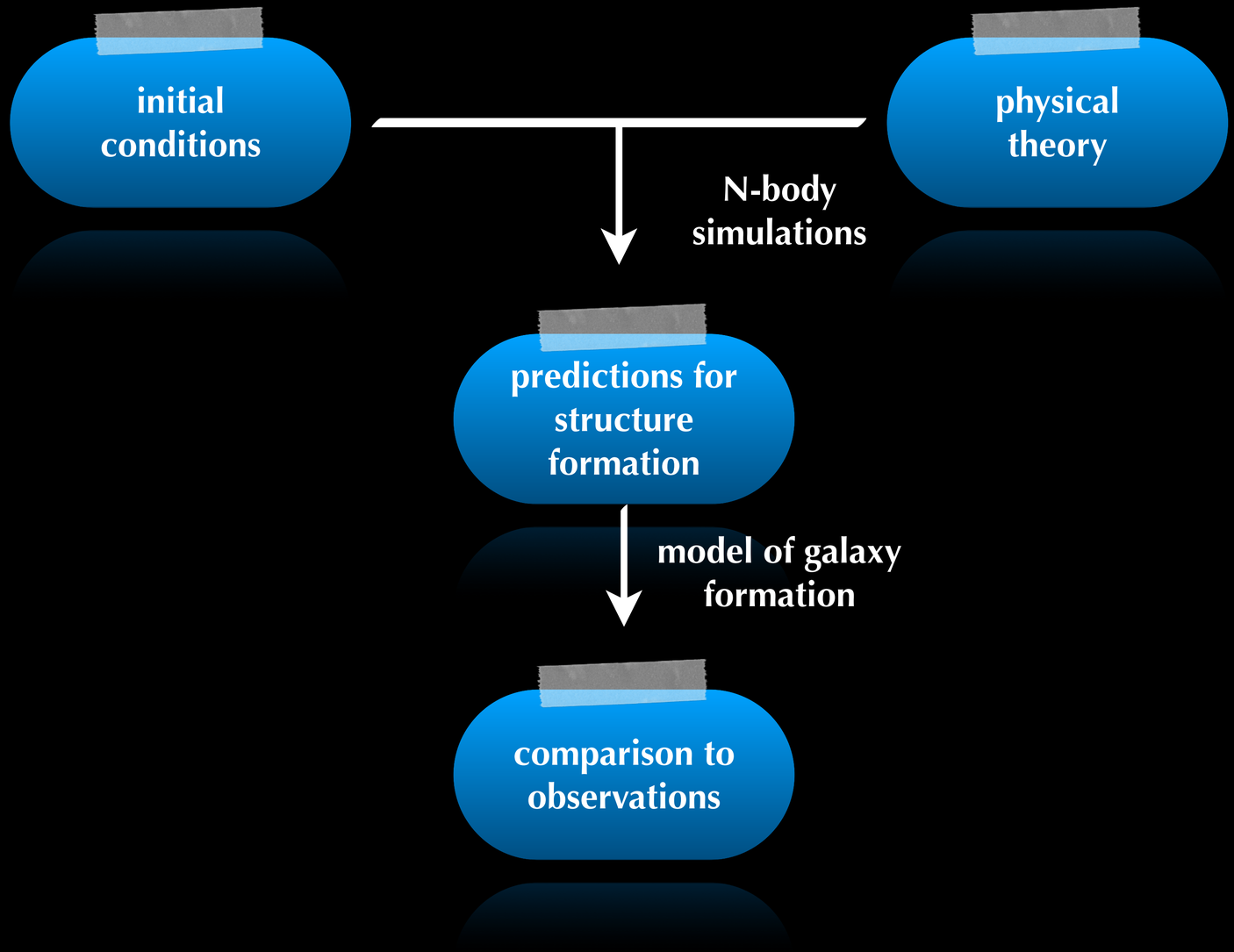
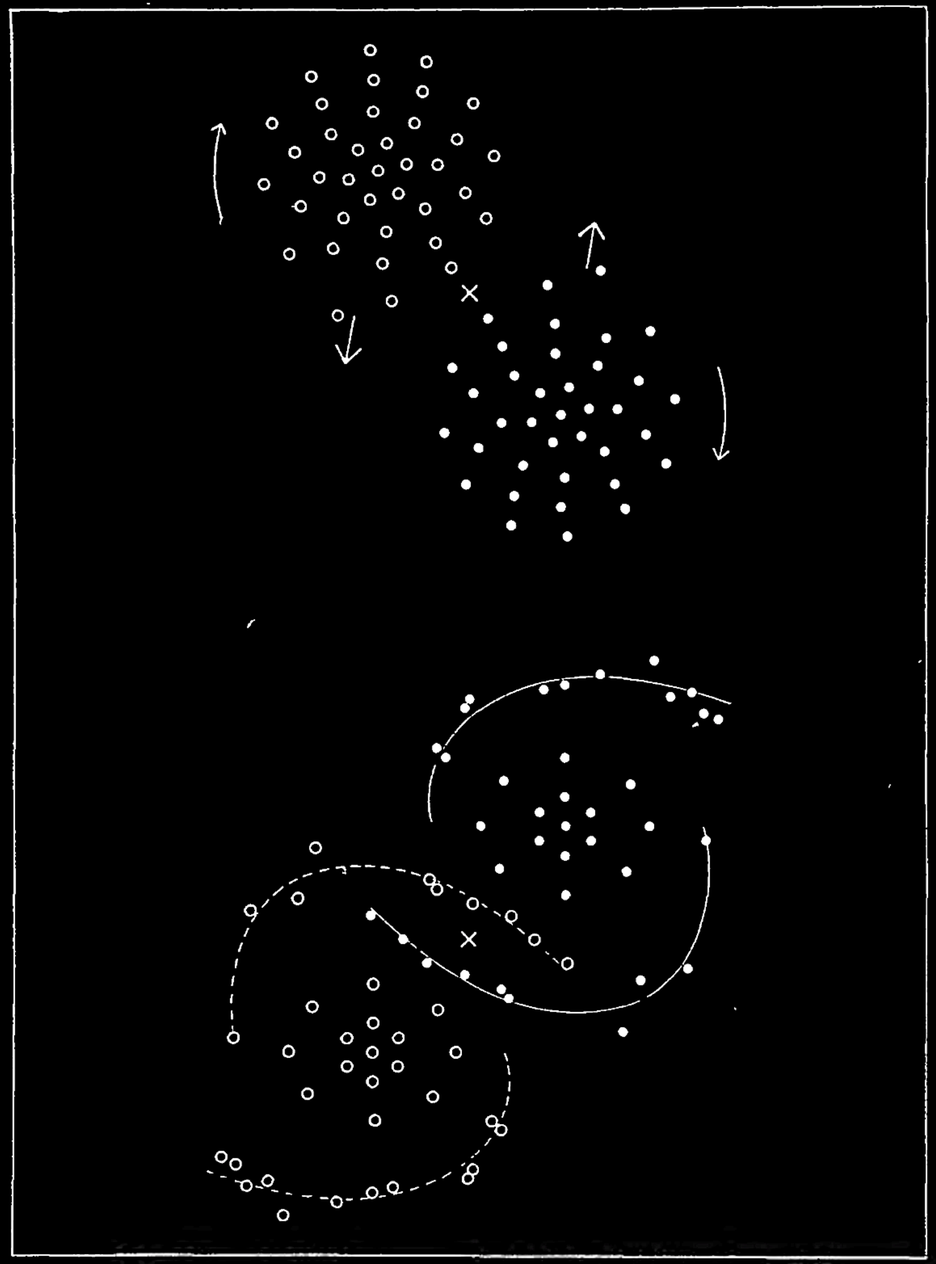


a little bit of history

Holmberg (1941)
the tidal encounter of two
“extragalactic nebulae”



White (1977);
700 particles

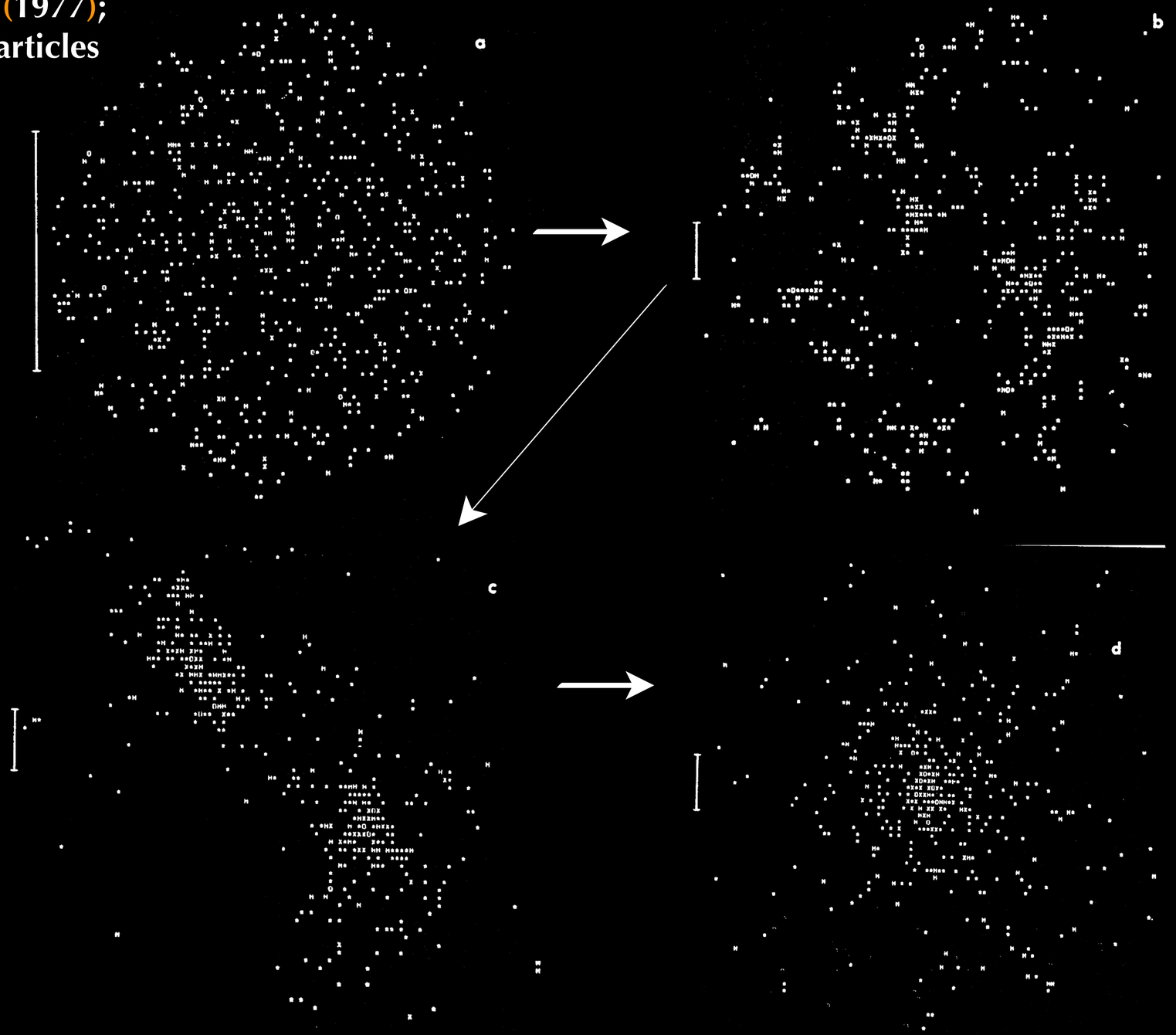


FIG. 1(c,d)

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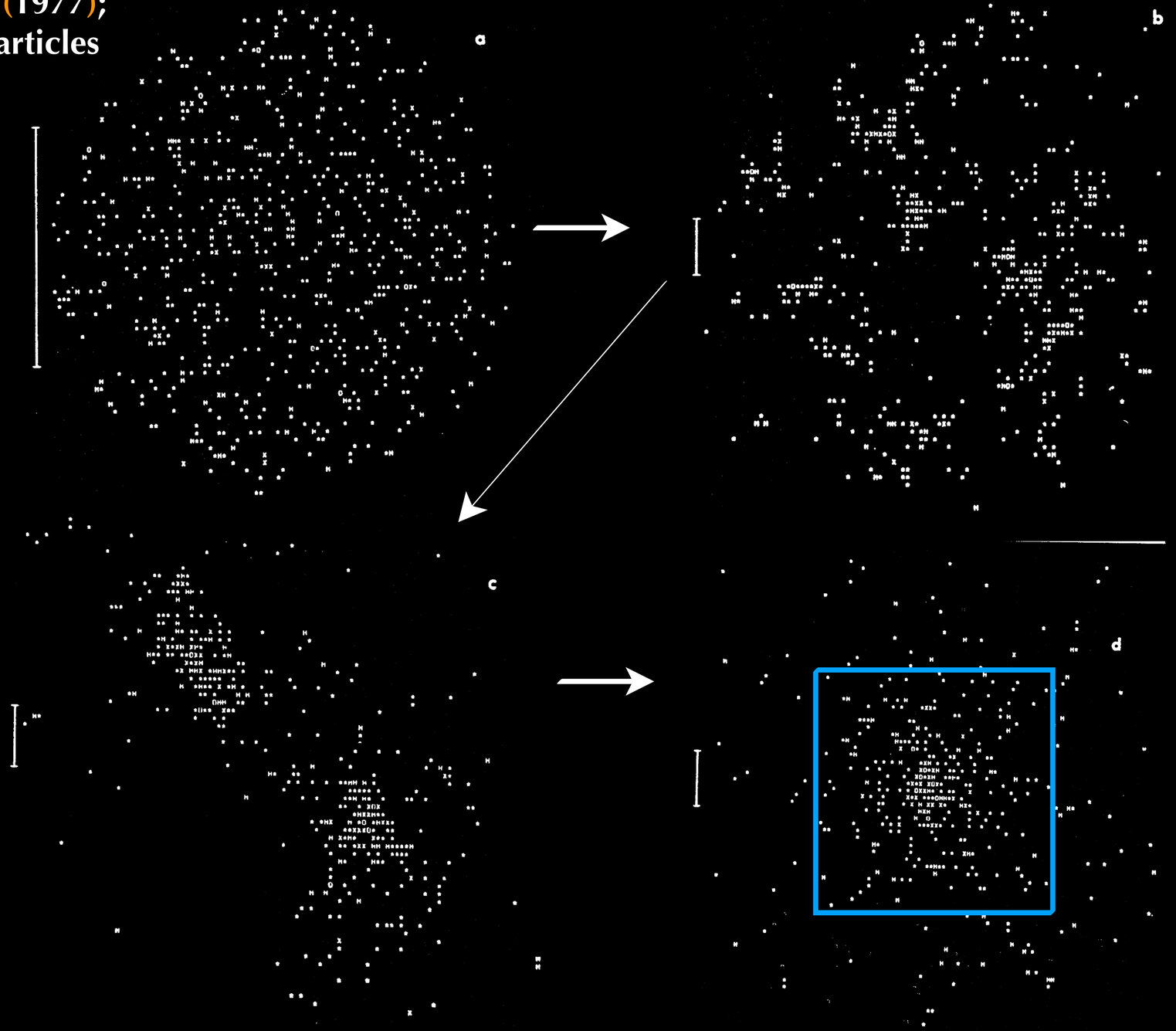
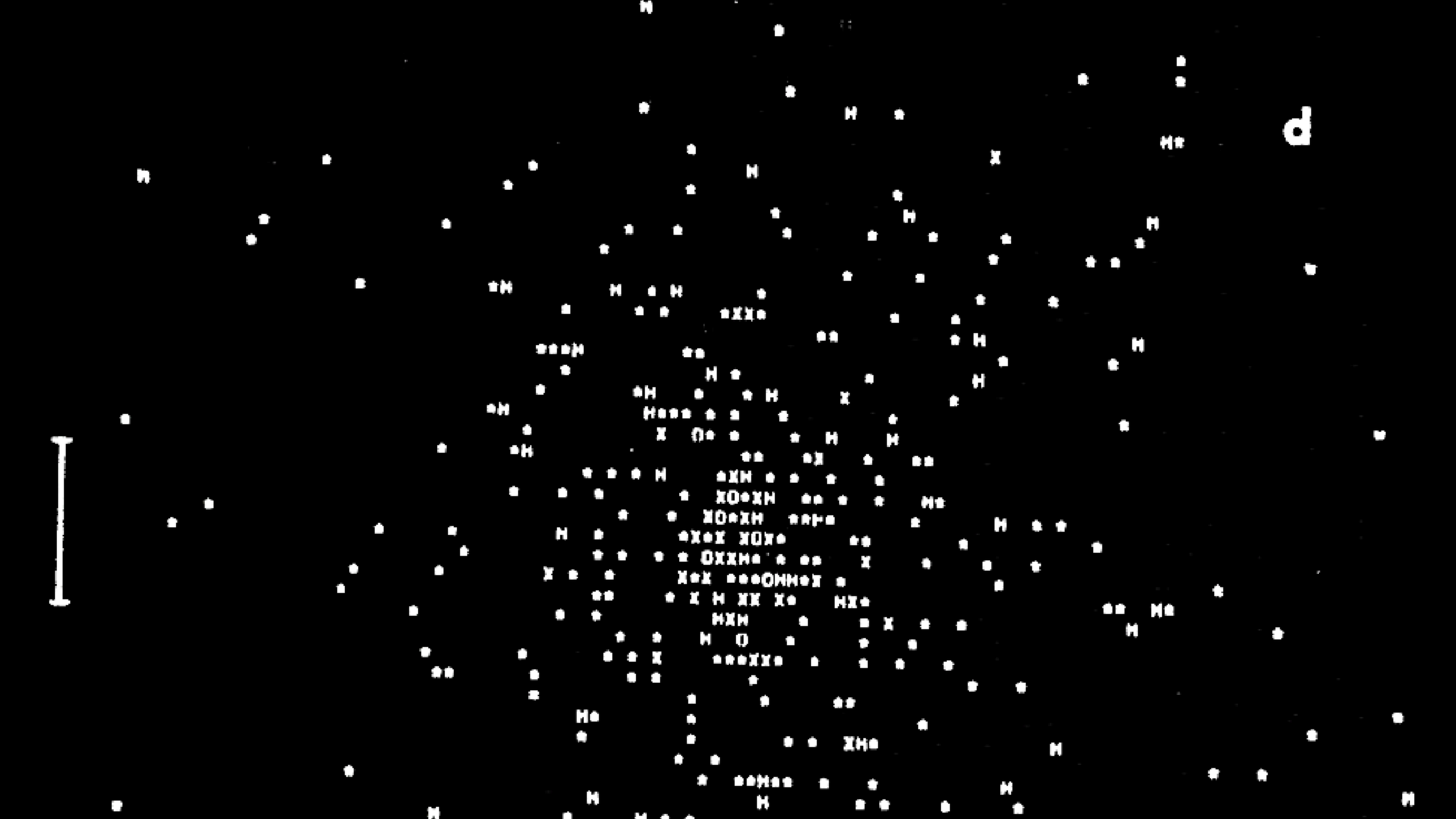


FIG. 1(c,d)


d

the rise of particle dark matter

Volume 94B, number 2 PHYSICS LETTERS 28 July 1980

AN ESTIMATE OF THE ν_e MASS FROM THE β-SPECTRUM OF TRITIUM IN THE VALINE MOLECULE

V.A. LUBIMOV, E.G. NOVIKOV, V.Z. NOZIK, E.F. TRETYAKOV and V.S. KOSIK [1]
Institute of Theoretical and Experimental Physics, Moscow, USSR

Received 4 June 1980

The high energy part of the β-spect
by a toroidal β-spectrometer. The resu

$14 \leqslant M_\nu \leqslant 46$ eV (99% C.L.).

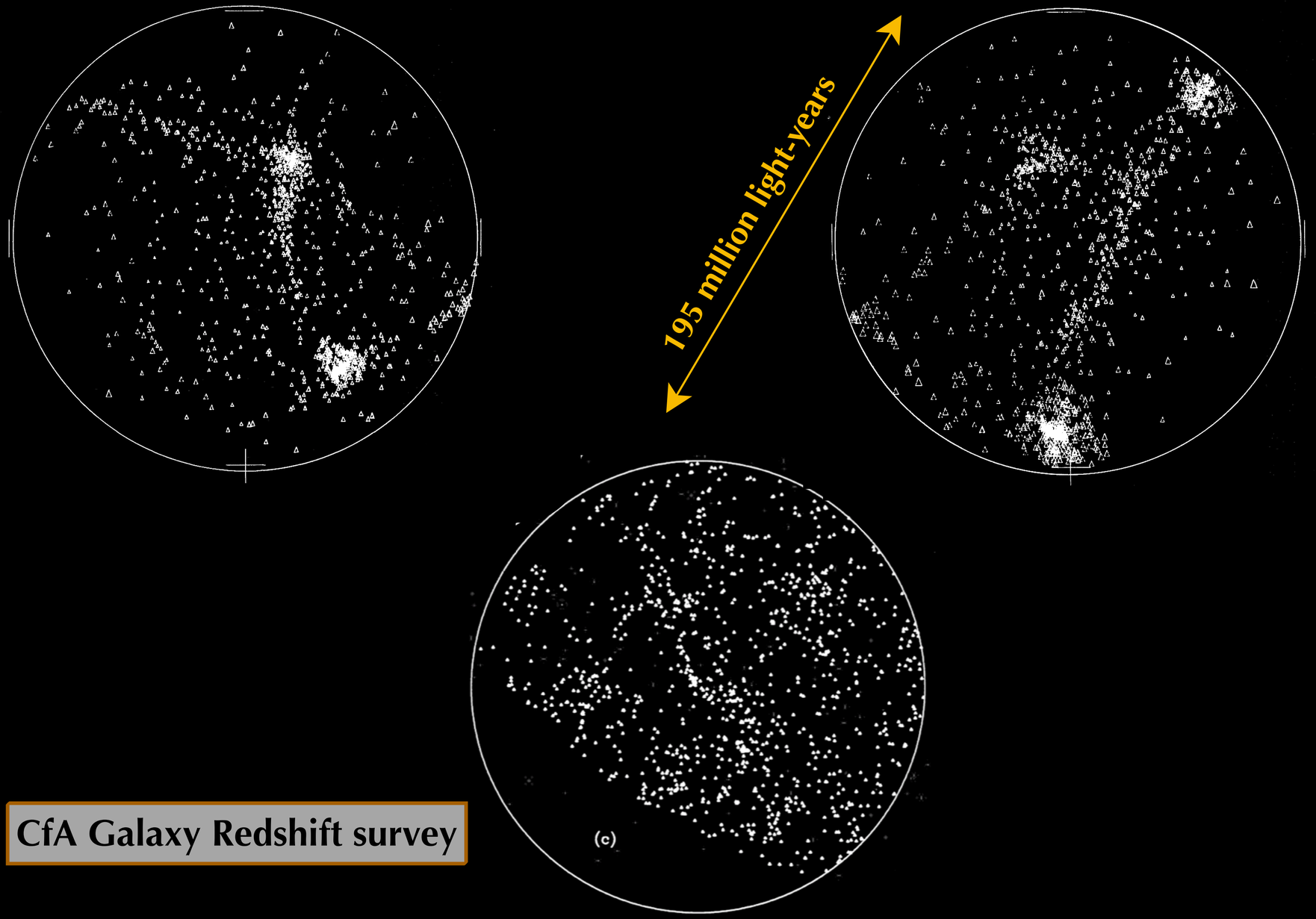
We consider this as an indication that the electron antineutrino has a non-zero mass. For the time being we do not see any effects which could have shifted essentially the above-mentioned limits. We continue the experimental study of the β-spectrum of tritium.

early candidates: the neutrino (~1980s)

weak interactions ✓ not visible ✓ known particle ✓

neutrinos are (almost) massless — zip around the Universe near the speed of light

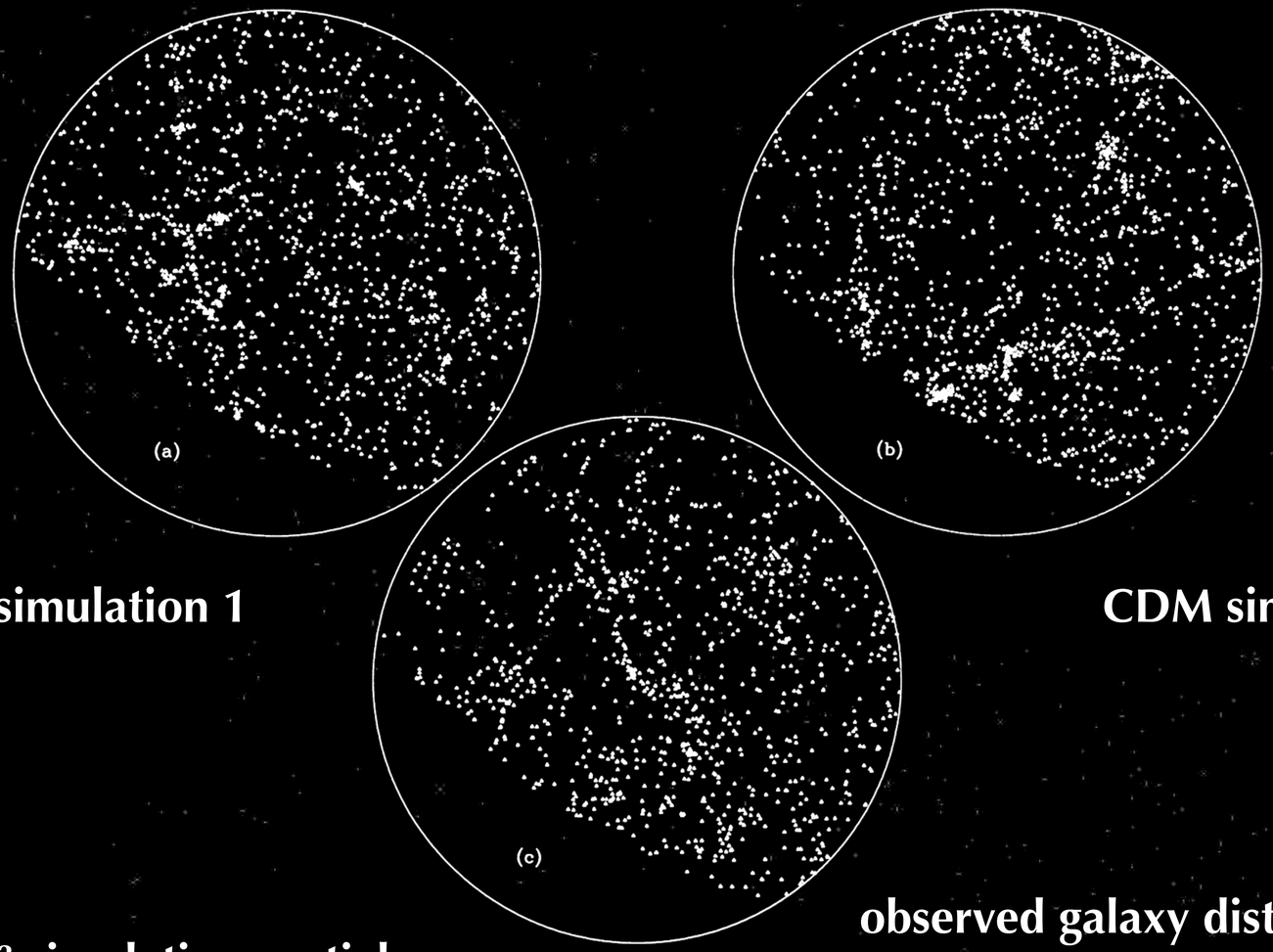
hot dark matter



CfA Galaxy Redshift survey

Klypin & Shandarin (1983); 32^3 simulation particles

the emergence of cold dark matter

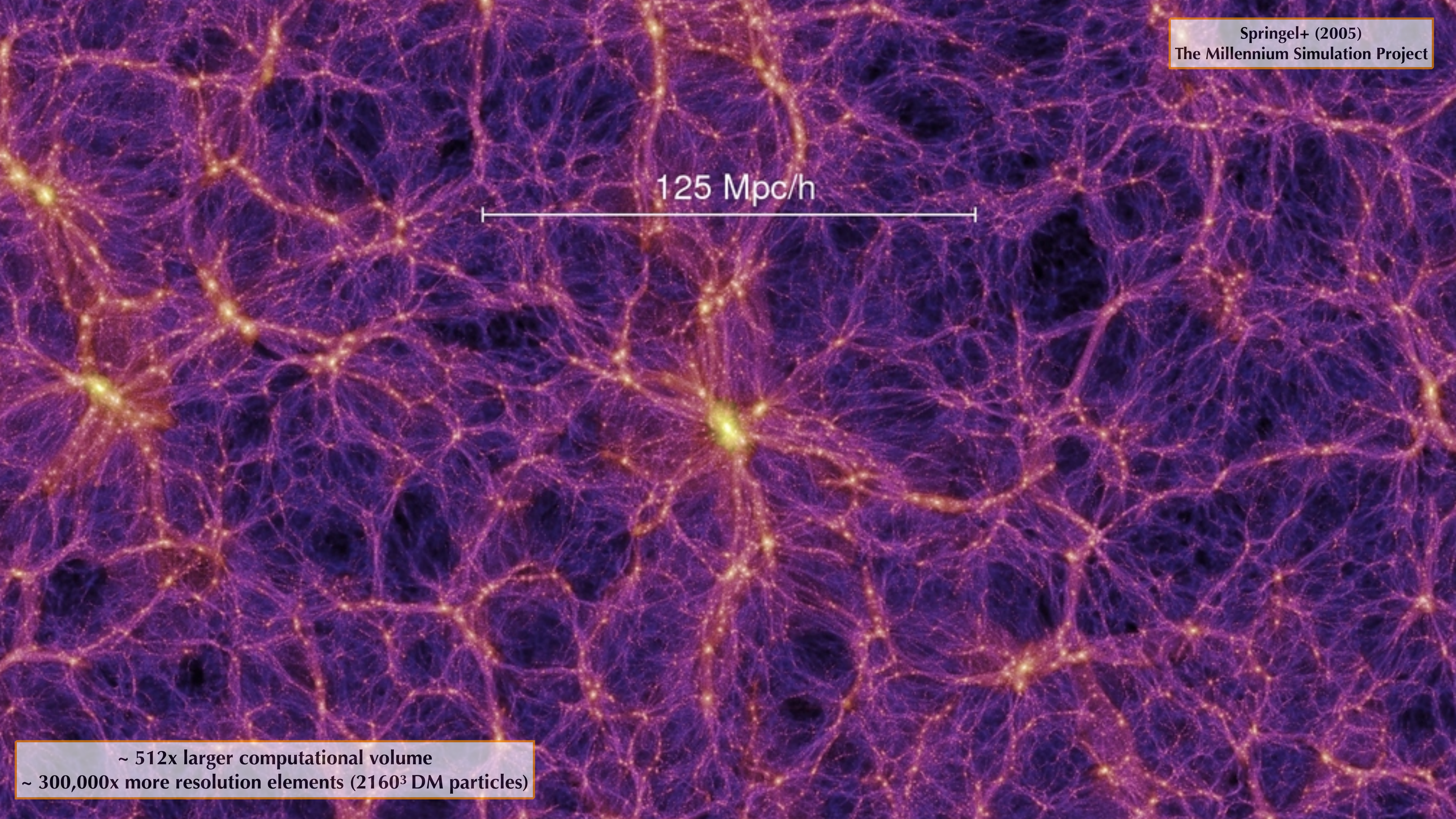


CDM simulation 1

CDM simulation 2

observed galaxy distribution

Davis+ (1985); 32^3 simulation particles



Springel+ (2005)
The Millennium Simulation Project

~ 512x larger computational volume
~ 300,000x more resolution elements (2160^3 DM particles)

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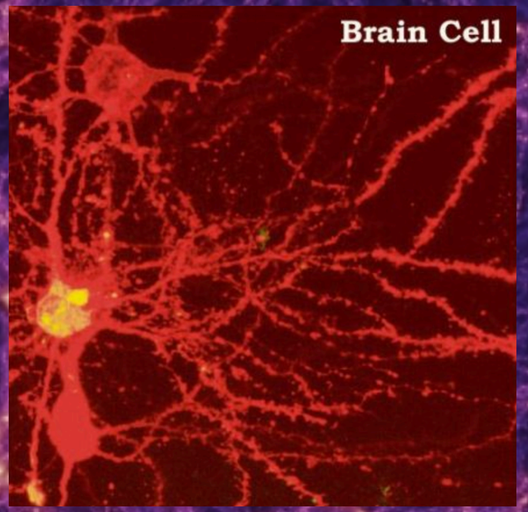
125 Mpc/h



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z = 48.4
T = 0.05 Gyr
500 kpc


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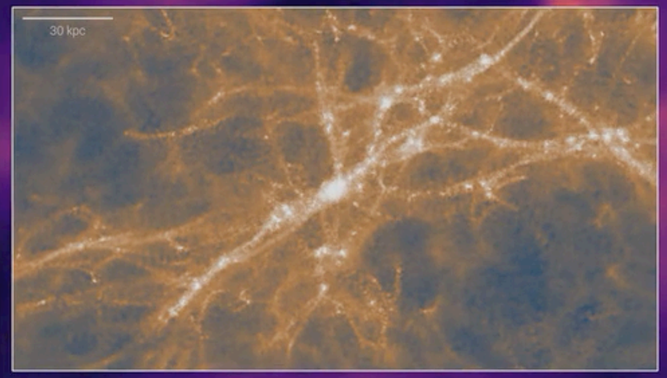
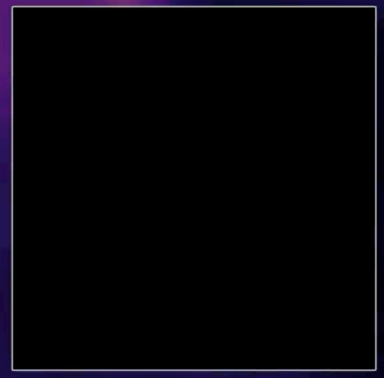
9 kpc

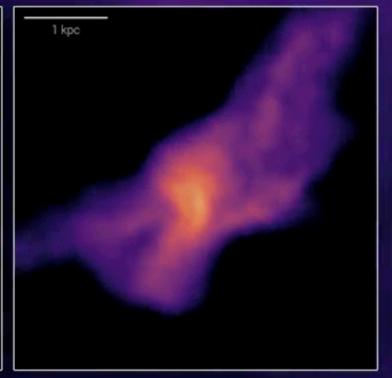
z = 9.8

log $M_\star$ = 7.74

SFR = 0.2 $M_\odot$ yr^{-1}







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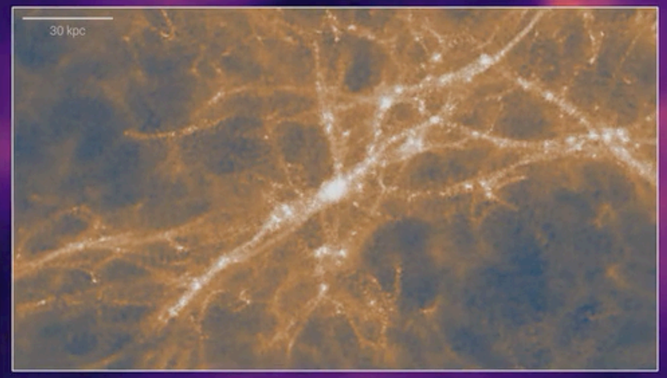

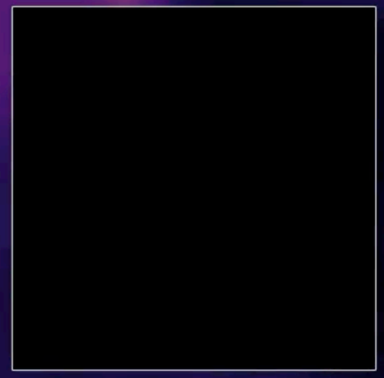

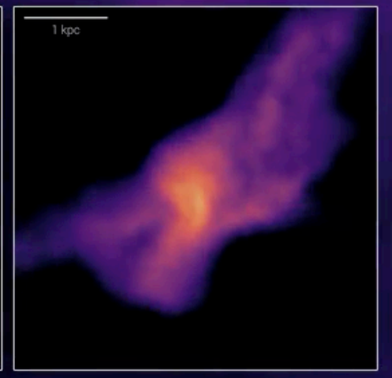

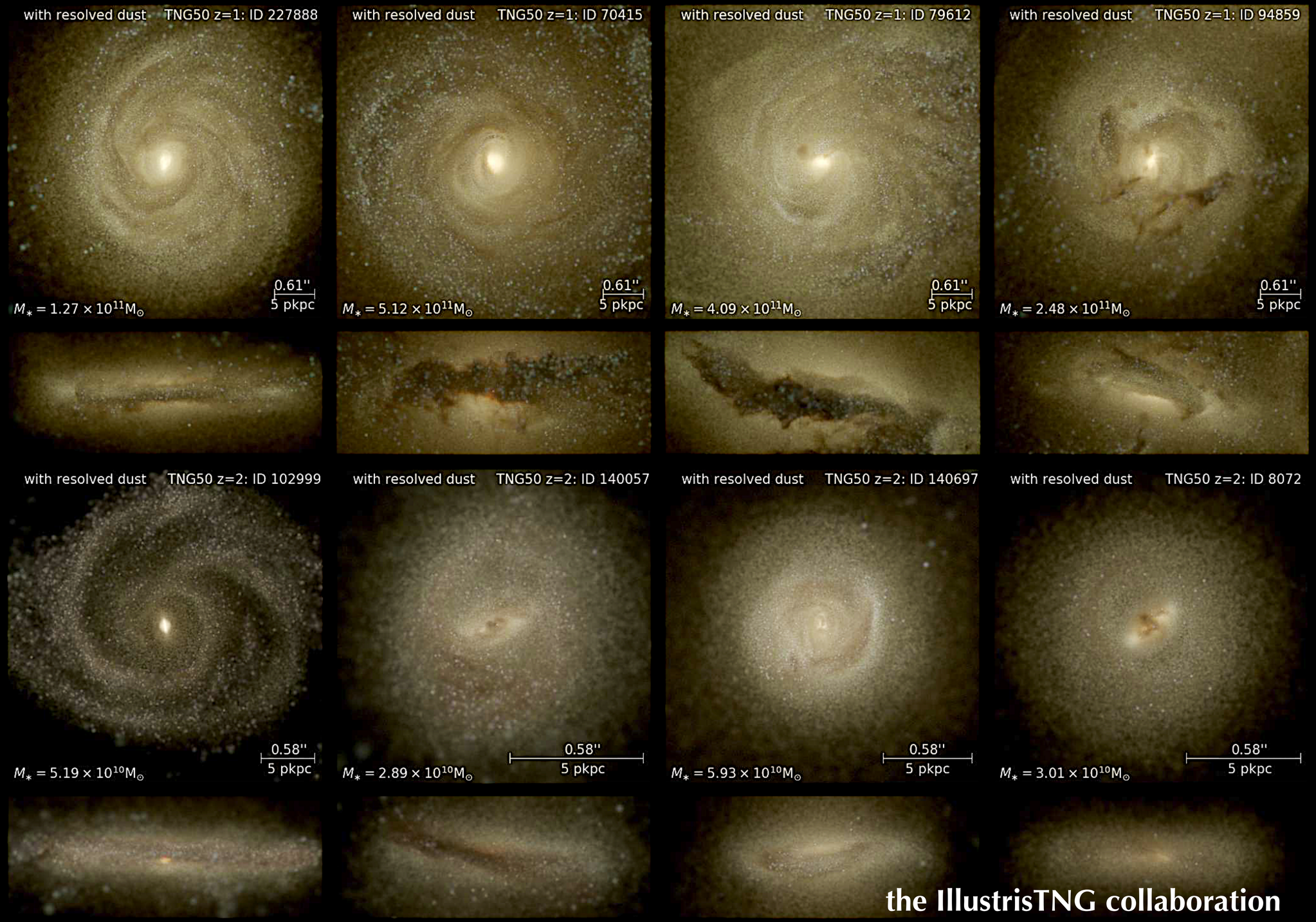
with resolved dust TNG50 z=1: ID 227888
$M_* = 1.27 \times 10^{11} M_\odot$
0.61''
5 pkpc
with resolved dust TNG50 z=1: ID 70415
$M_* = 5.12 \times 10^{11} M_\odot$
0.61''
5 pkpc
with resolved dust TNG50 z=1: ID 79612
$M_* = 4.09 \times 10^{11} M_\odot$
0.61''
5 pkpc
with resolved dust TNG50 z=1: ID 94859
$M_* = 2.48 \times 10^{11} M_\odot$
0.61''
5 pkpc
with resolved dust TNG50 z=2: ID 102999
$M_* = 5.19 \times 10^{10} M_\odot$
0.58''
5 pkpc
with resolved dust TNG50 z=2: ID 140057
$M_* = 2.89 \times 10^{10} M_\odot$
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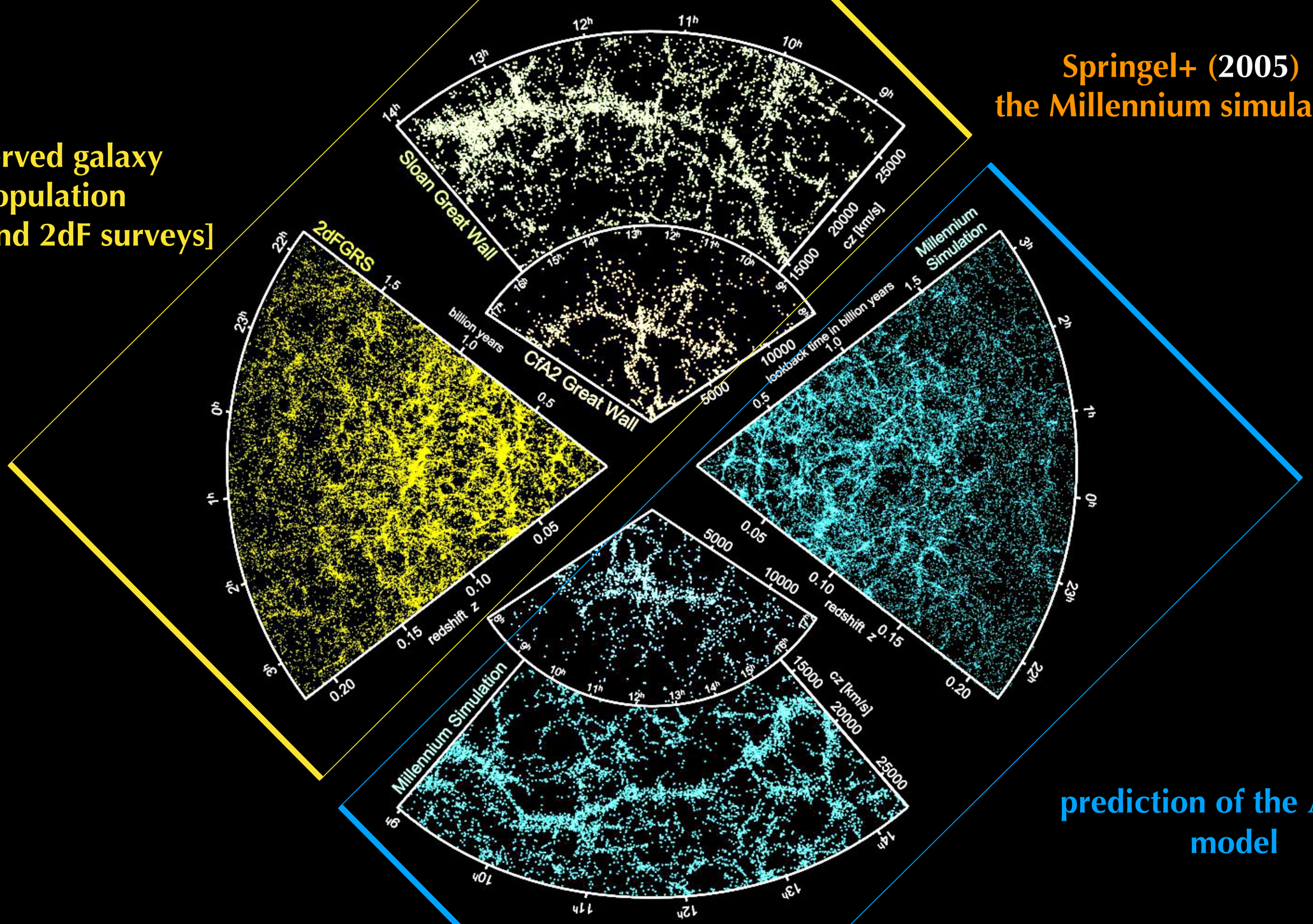
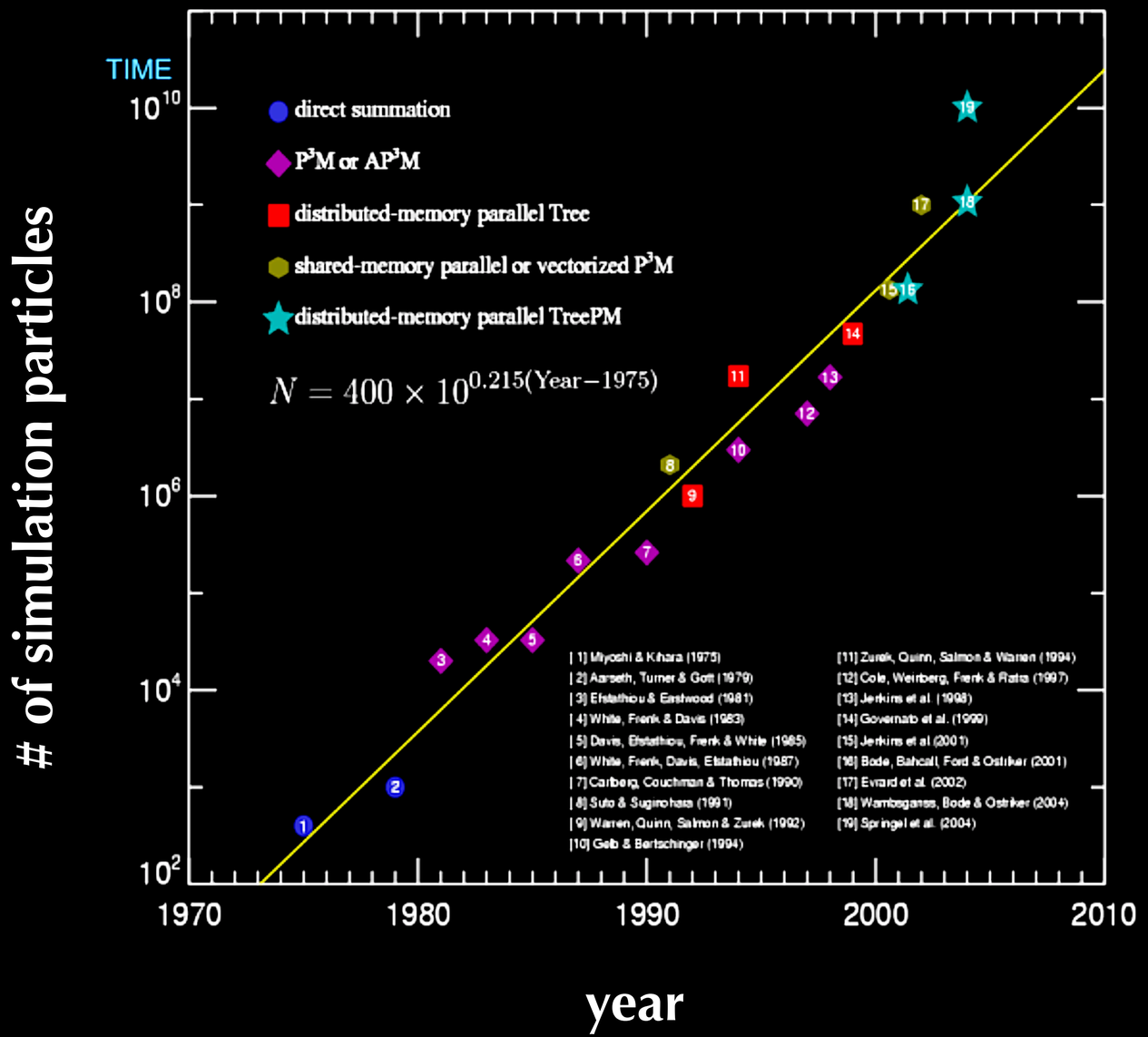
5 pkpc
with resolved dust TNG50 z=2: ID 140697
$M_* = 5.93 \times 10^{10} M_\odot$
0.58''
5 pkpc
with resolved dust TNG50 z=2: ID 8072
$M_* = 3.01 \times 10^{10} M_\odot$
0.58''
5 pkpc
the IllustrisTNG collaboration

observed galaxy population [SDSS and 2dF surveys]

Springel+ (2005) the Millennium simulation

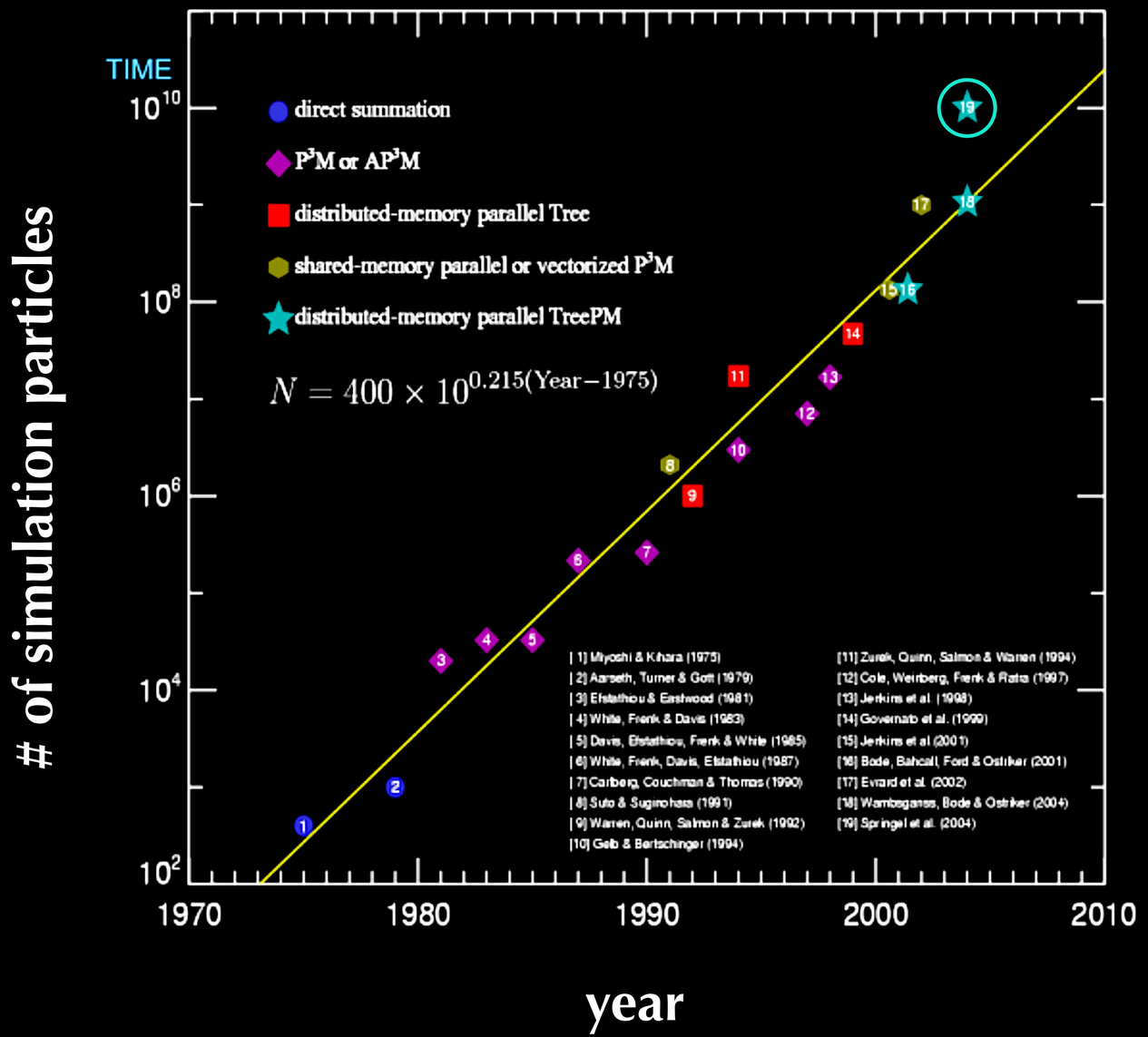


prediction of the ΛCDM model



Moore's Law — computers double their speed every ~18 months or so

N-body simulations have roughly doubled in size every 16-17 months



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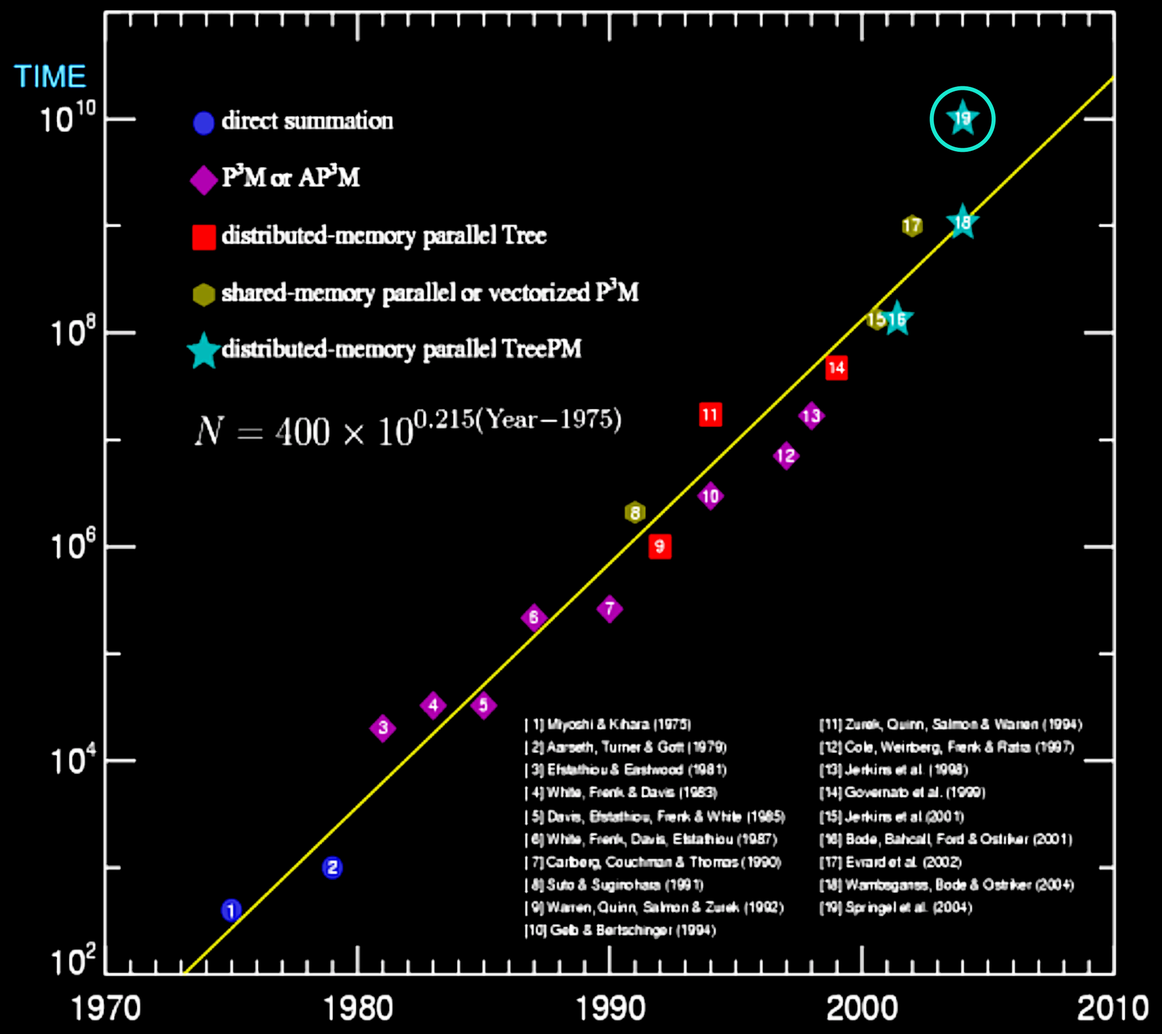

2017
[Euclid Flagship]

2016
[OuterRim]

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the N-body method

Poisson-Vlasov equation [fluid]

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \left(-\frac{\partial \Phi}{\partial \mathbf{x}} \right) = 0$$

$$\nabla^2 \Phi(\mathbf{x}, t) = 4\pi G \int f(\mathbf{x}, \mathbf{v}, t)\, \mathrm{d}\mathbf{v}$$

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macroscopic DM [particles]

$$\ddot{\mathbf{x}}_i = -\nabla_i \Phi(\mathbf{x}_i)$$

$$\Phi(\mathbf{x}) = -G \sum_{j=1}^{N} \frac{m_j}{\left[\left(\mathbf{x} - \mathbf{x}_j \right)^2 + \epsilon^2 \right]^{1/2}}$$

sample the phase-space of dark matter with macroscopic particles

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→ need large N to be valid!

relaxation time in an N-body system

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velocity dispersion

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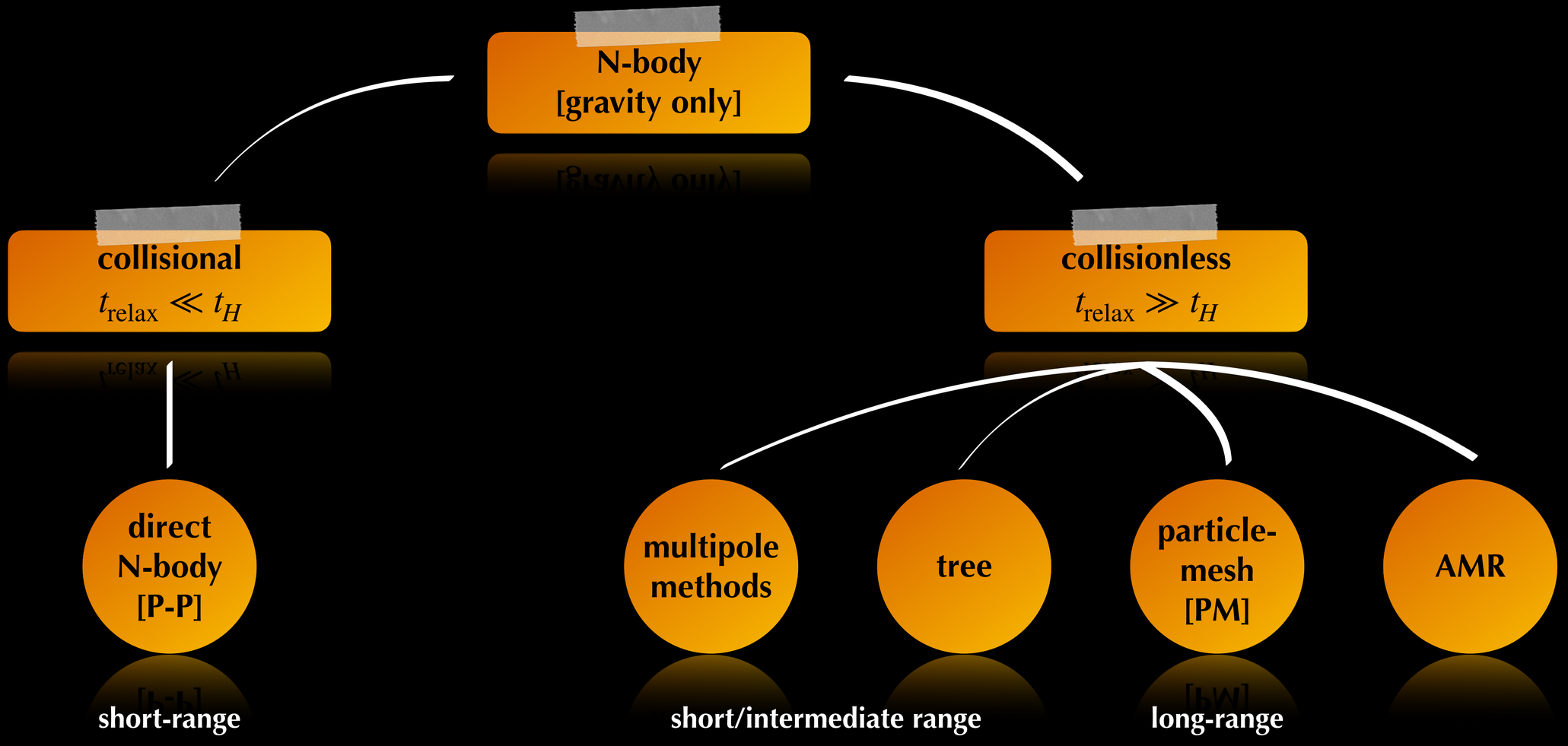
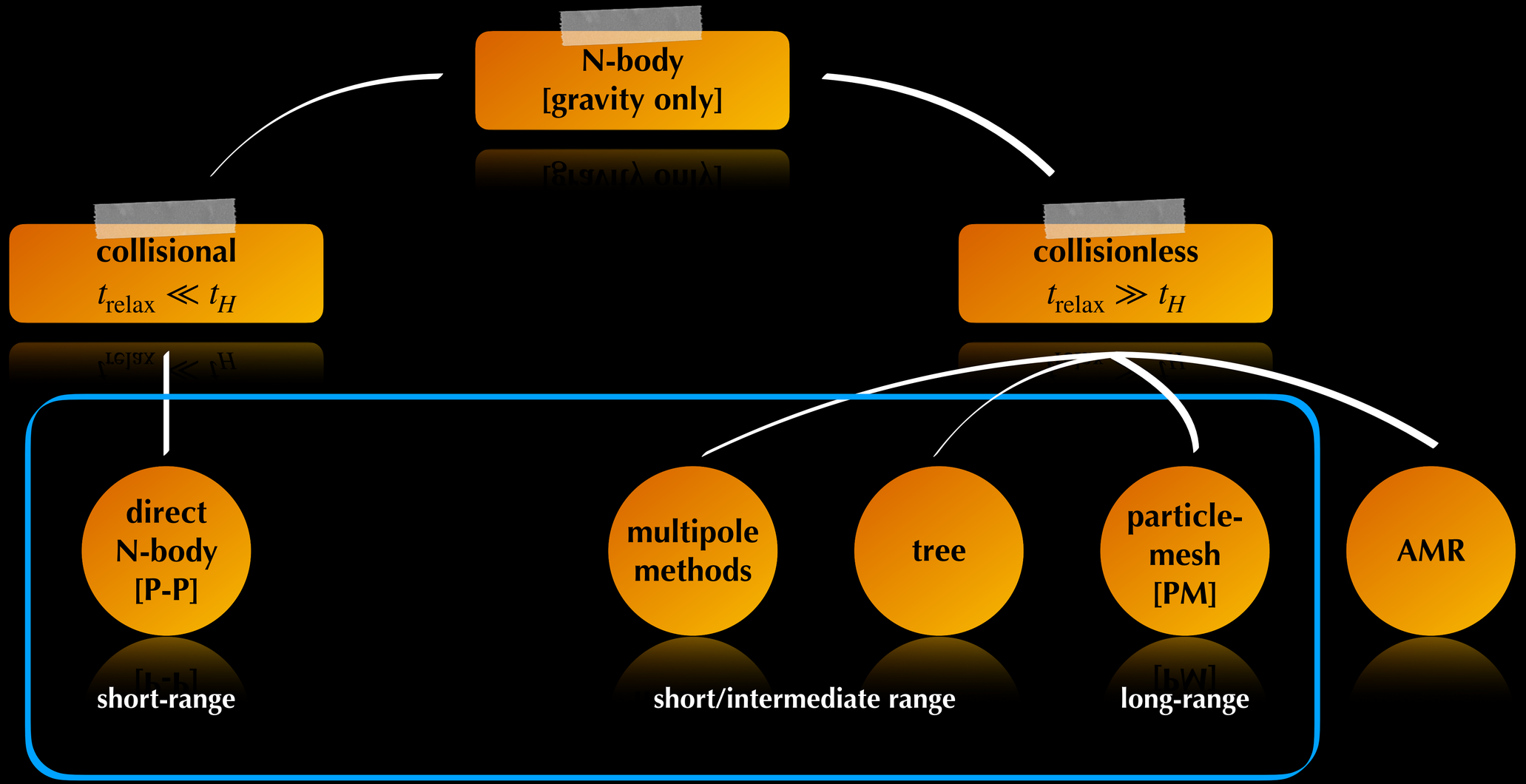
characteristic size of system

velocity dispersion

in a "real" dark matter halo, $N \sim 10^{70}$, so we can always treat it as a collision less system. in a simulation, typically $N \sim 10^9$, so relaxation timescale is dramatically shorter

$t_{\rm relax} \gg t_H$ collisionless


N-body
[gravity only]
collisional
$t_{\text{relax}} \ll t_H$
collisionless
$t_{\text{relax}} \gg t_H$
direct
N-body
[P-P]
multipole
methods
tree
particle-
mesh
[PM]
AMR
short-range
short/intermediate range
long-range



hybrid methods: GADGET, SWIFT, PKDgrav

direct N-body: particle-particle method

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this is the simplest N-body algorithm one can cook up: simply compute the force on particle j due to all $N-1$ other particles, and repeat over all particles

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super-easy to understand
general
highly accurate

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direct N-body: particle-particle method

$$\ddot{x}_i = -\nabla\Phi(x_i)$$

$$\Phi(x) = -G\sum_{j=1}^{N}\frac{m_j}{\left[\left(\mathbf{x}-\mathbf{x}_j\right)^2+\epsilon^2\right]^{1/2}}$$

super-easy to understand

general

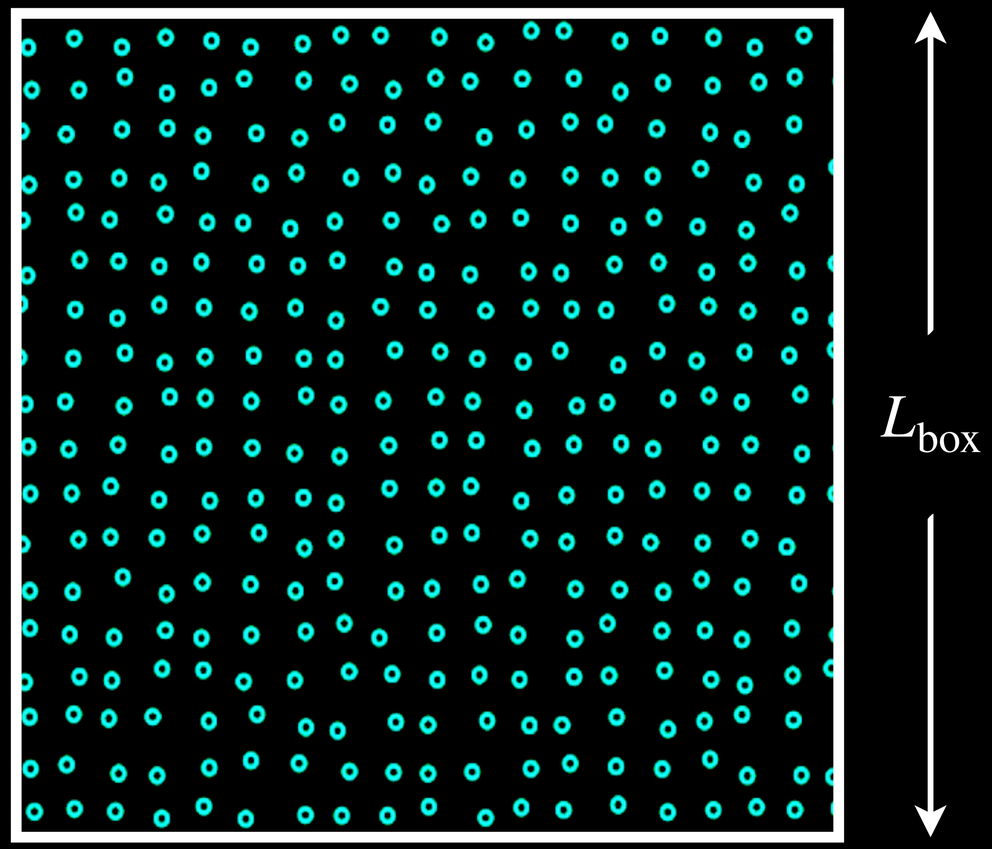
highly accurate

computationally *extremely* expensive

$\mathcal{O}(N^2)$

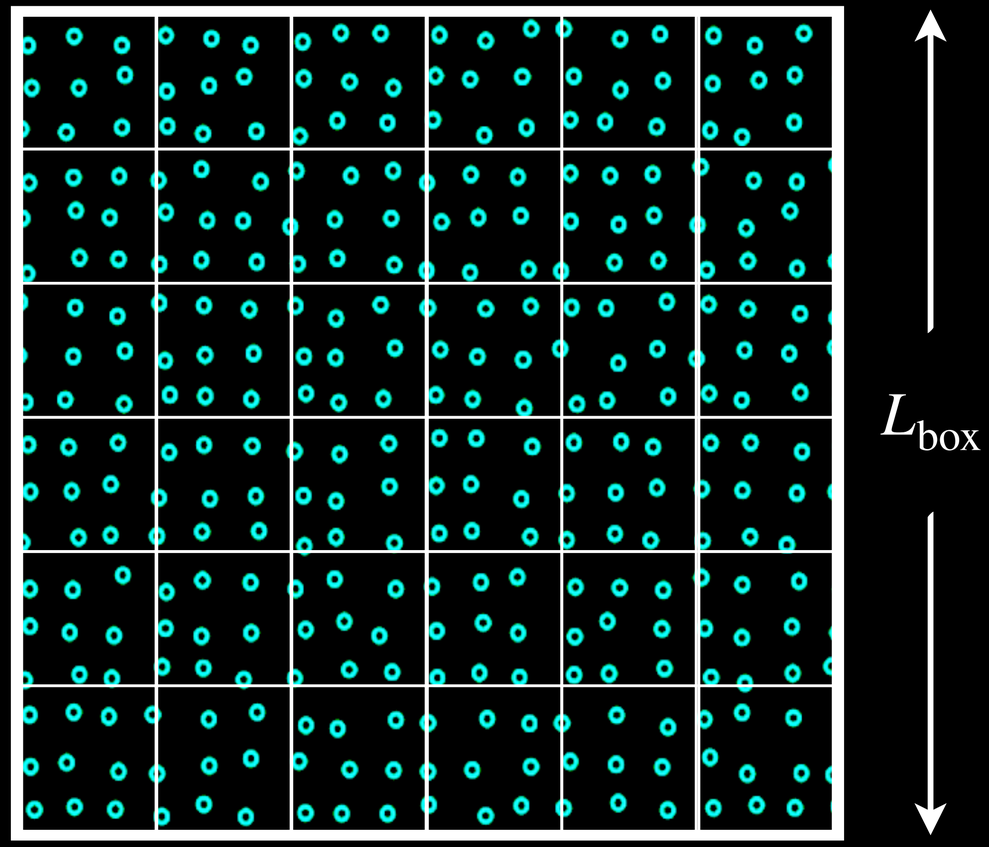
this is the simplest N-body algorithm one can cook up: simply compute the force on particle j due to all $N-1$ other particles, and repeat over all particles

particle-mesh method



use the properties of Fourier transforms + periodic boundary conditions to solve: $\Phi(\mathbf{k}) = G(\mathbf{k}) \cdot \rho(\mathbf{k})$

particle-mesh method



1. divide computational volume into a grid of size N_{cells} x N_{cells} x N_{cells}

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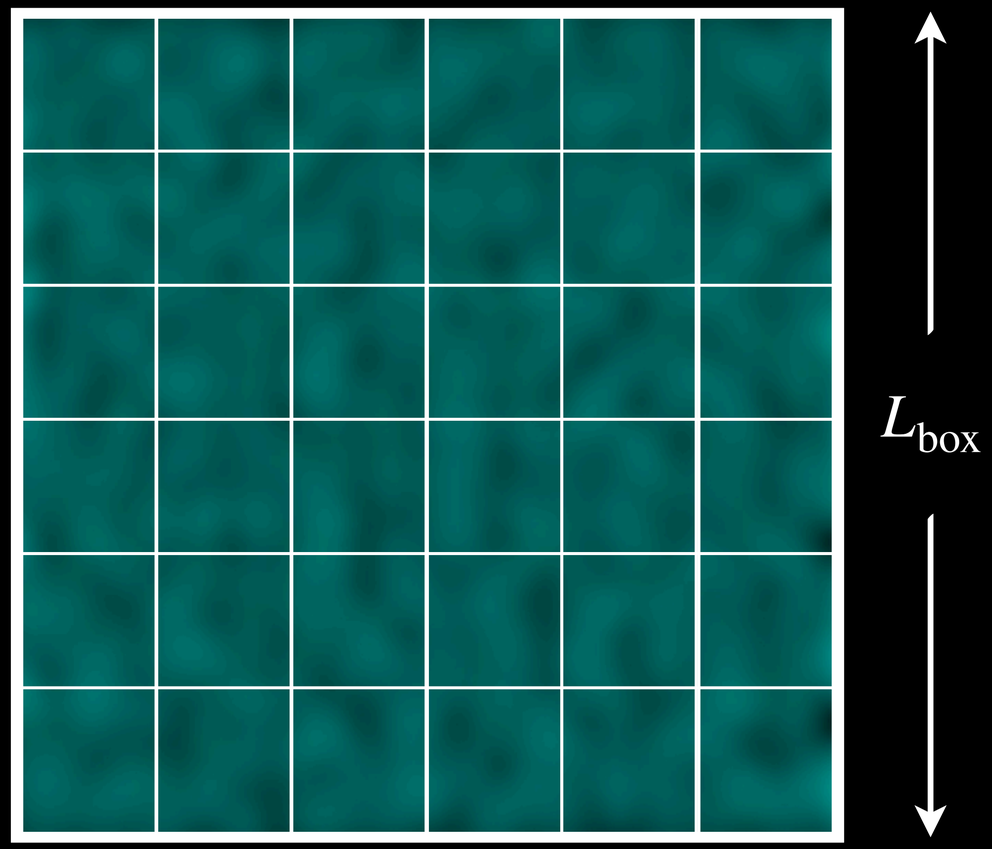

1. divide computational volume into a grid of size N_{cells} x N_{cells} x N_{cells}

2. smooth the discrete particle distribution onto mesh using an interpolation scheme (CIC, NGP, TSC etc): density field $\rho(\mathbf{x})$

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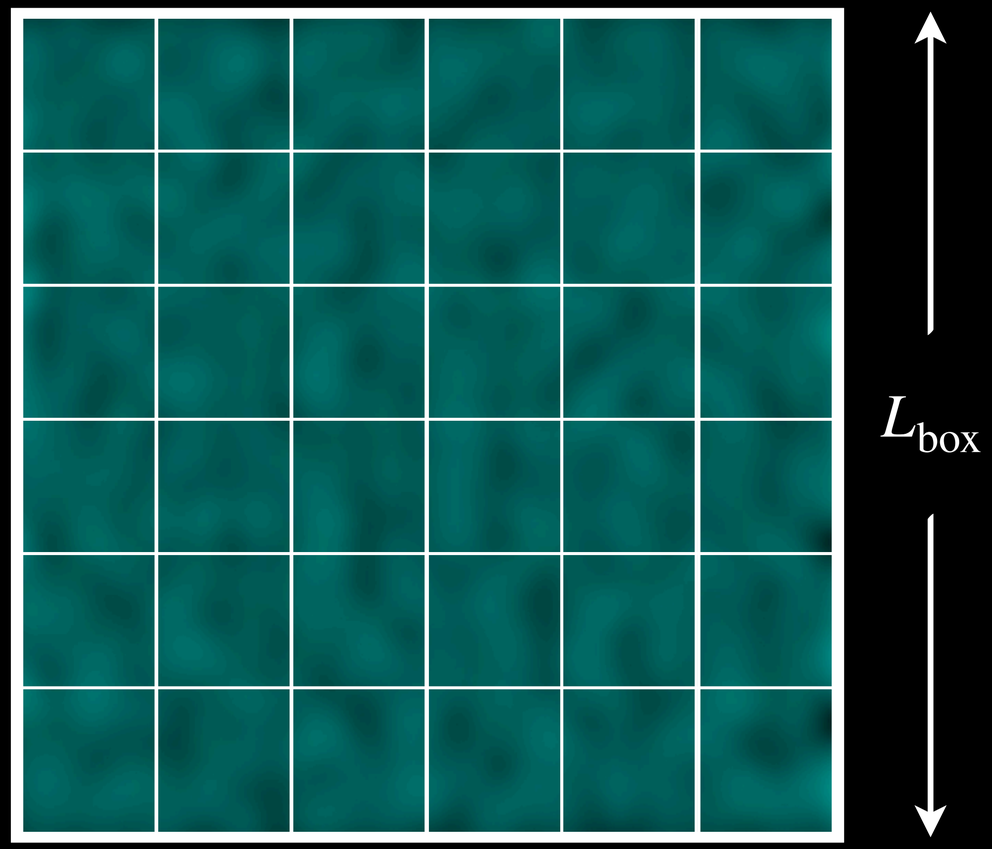

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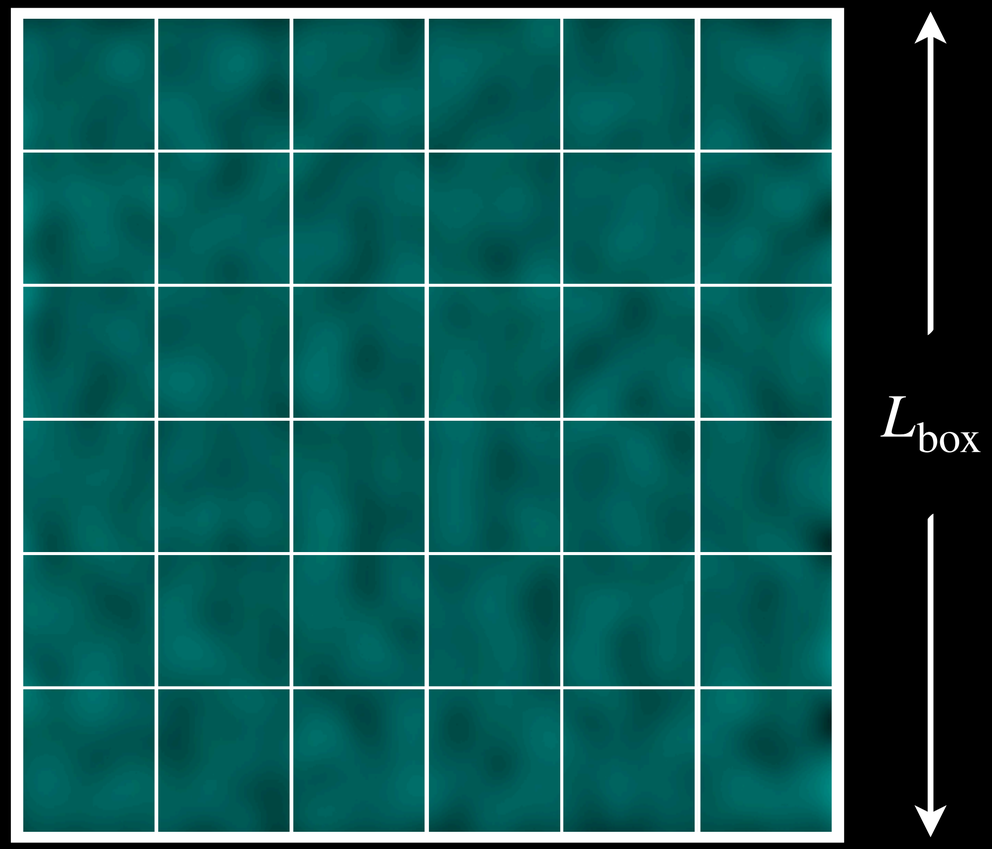

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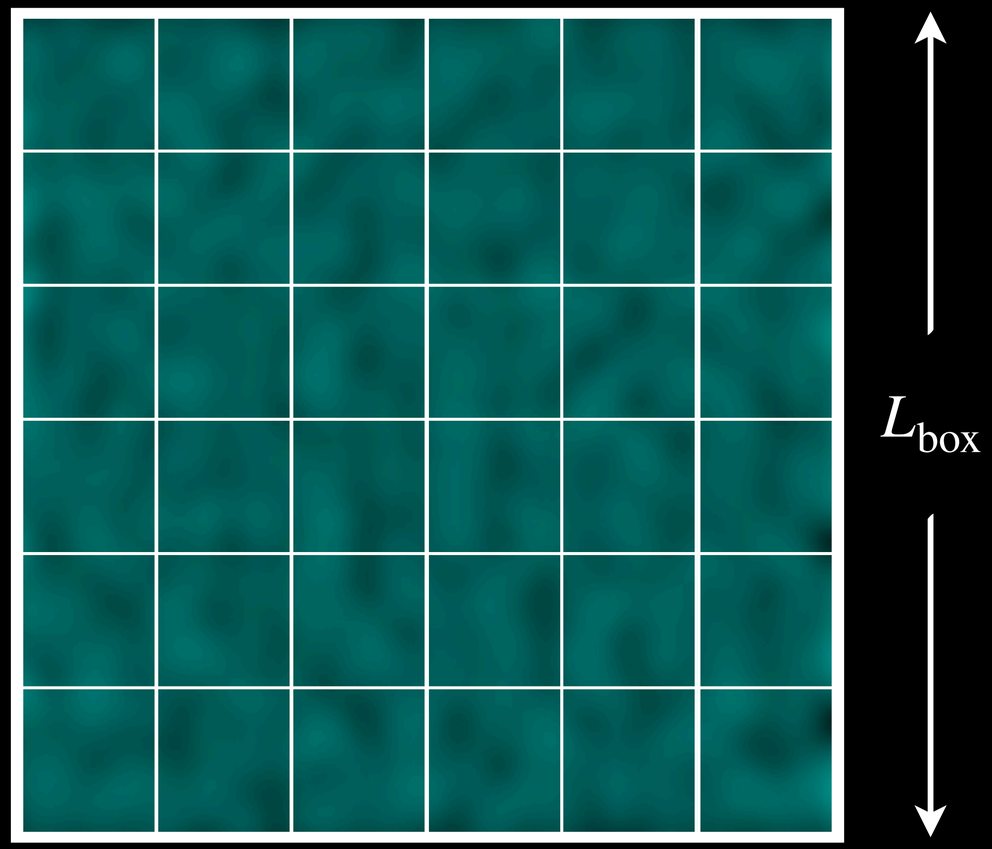

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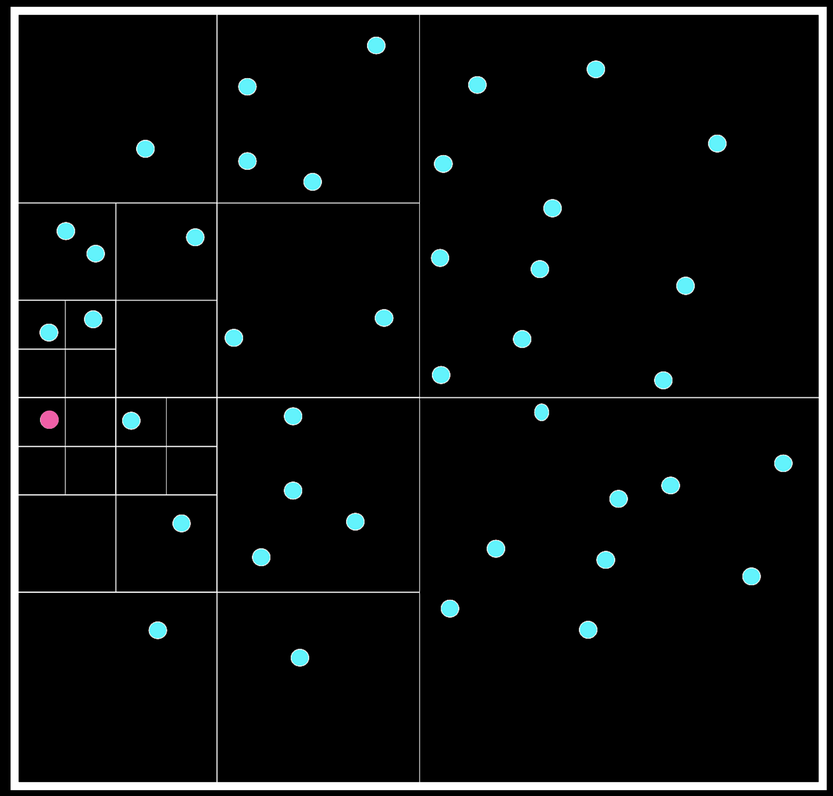
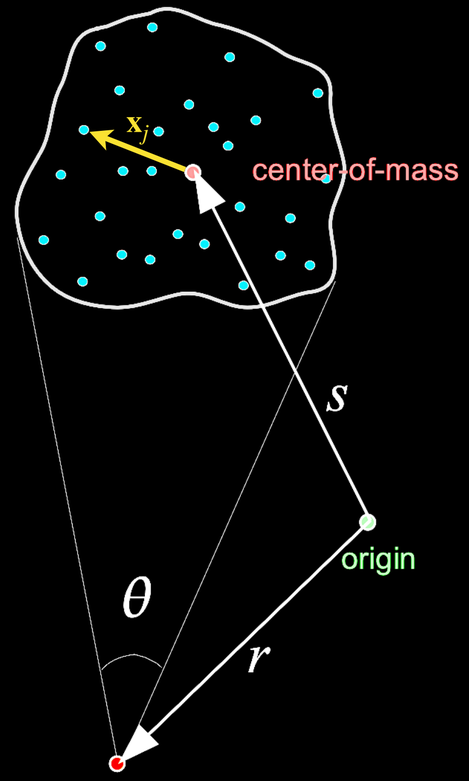
5. inverse Fourier transform to get $\Phi(\mathbf{x})$

use the properties of Fourier transforms + periodic boundary conditions to solve: $\Phi(\mathbf{k}) = G(\mathbf{k}) \cdot \rho(\mathbf{k})$

tree algorithms

based on the idea that you can group together particles that are a long way away from the particle of interest (pink)





Springel (2005)

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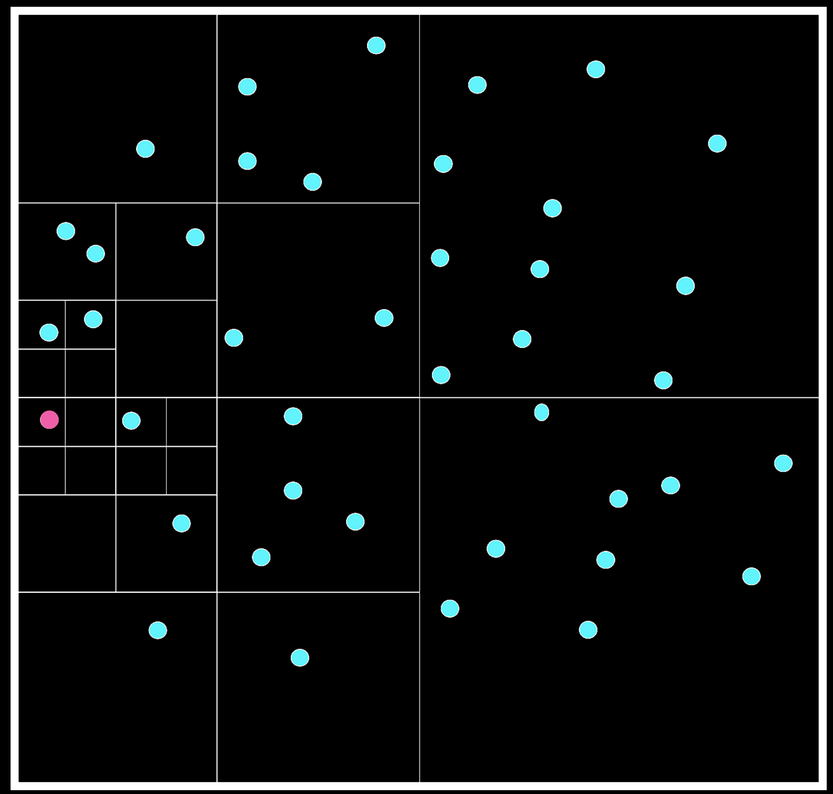

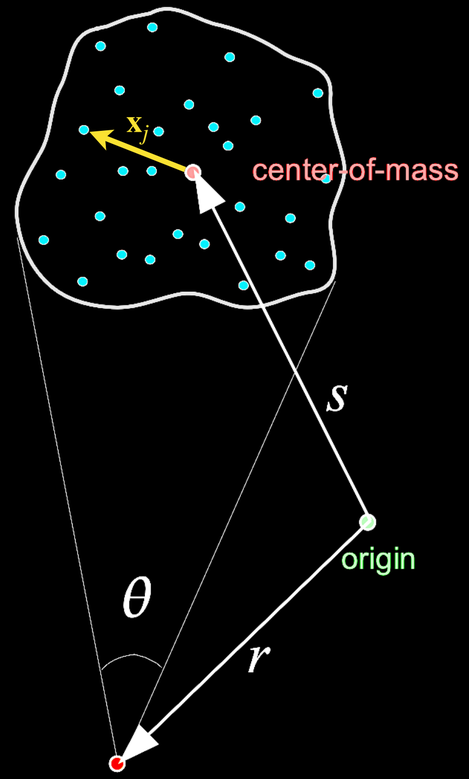

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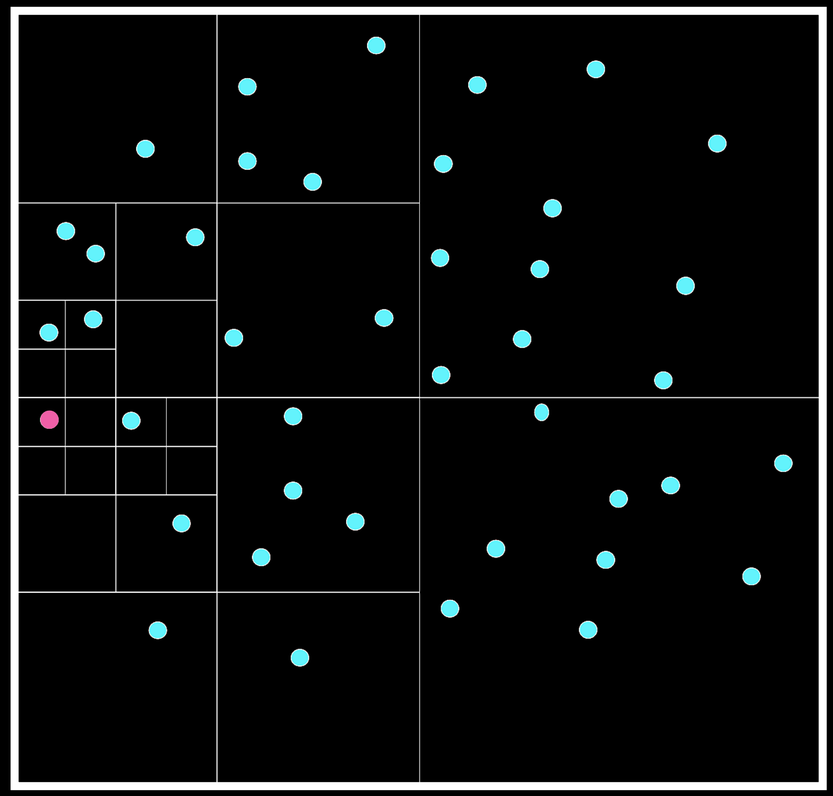

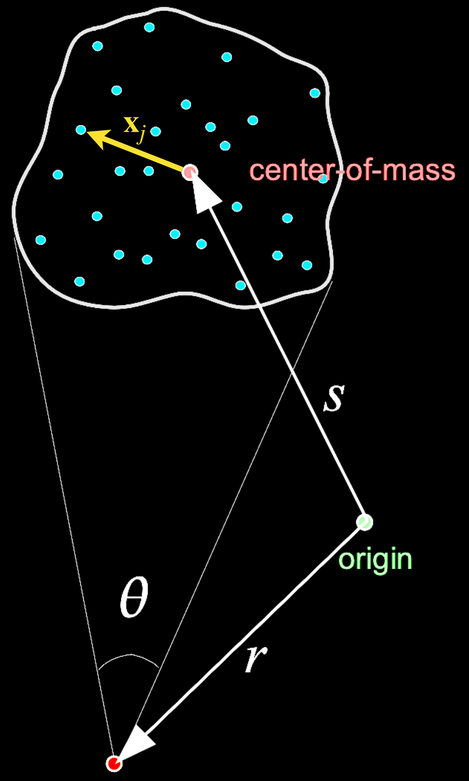

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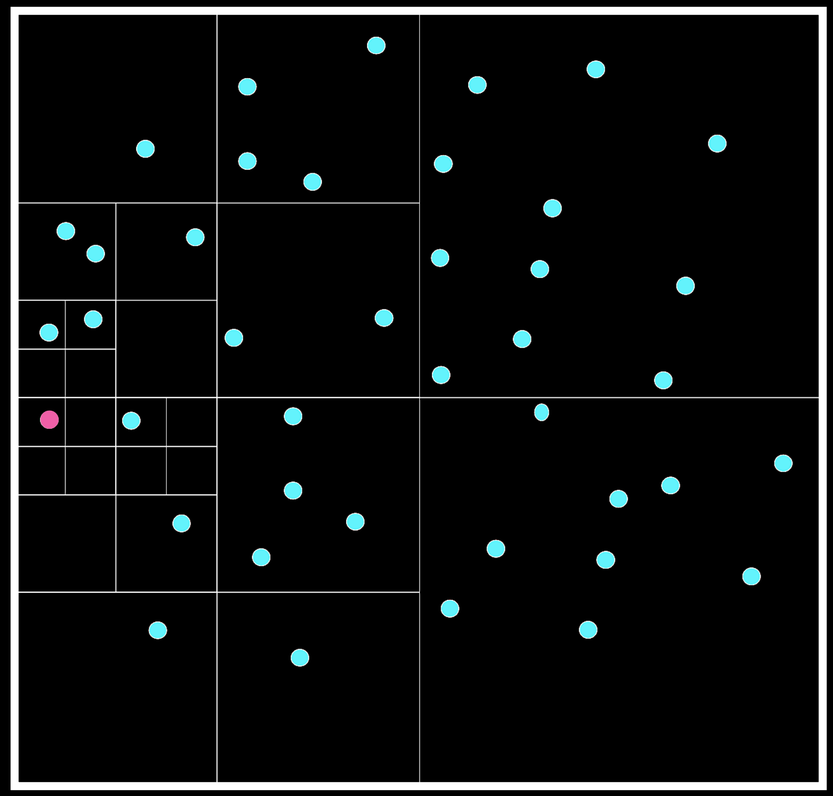
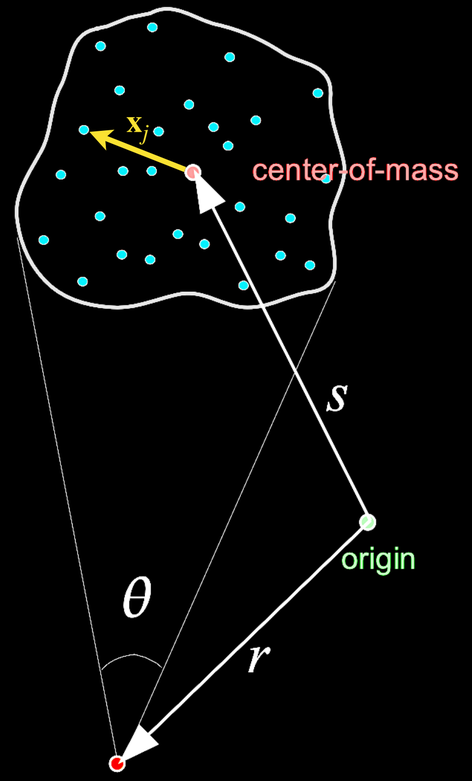


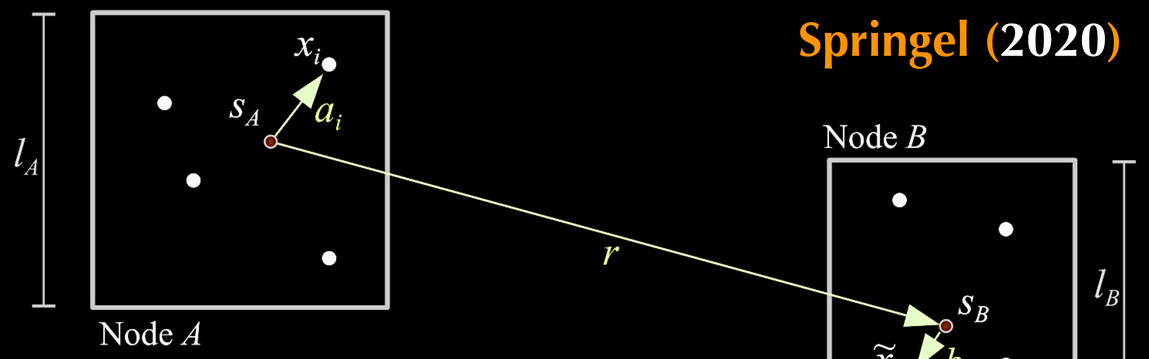


Springel (2005)

gravitational potential generated by points inside a node:

$$\Phi(\mathbf{x}) = -G \sum_{j \in \text{node}} m_j \, g\left(\tilde{\mathbf{x}}_j - \mathbf{x}\right)$$

fast multipole method



Springel (2020)

"sink"

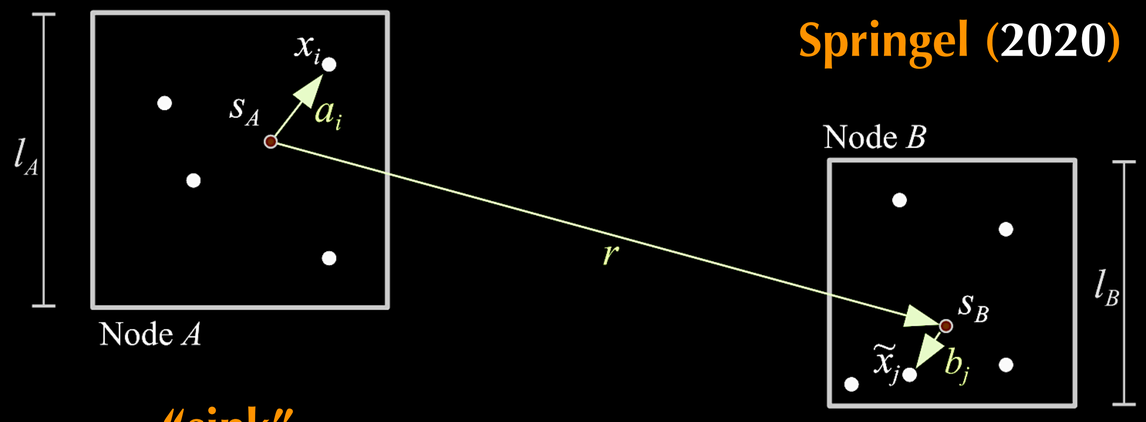
"source"

$$\Phi\left(\mathbf{x}_i\right) = -G \sum_j m_j \, g\left(\tilde{\mathbf{x}}_j - \mathbf{x}_i\right)$$

the fast multipole method (FMM) is arguably the most efficient way to compute hierarchical multipole expansions of the gravitational potential with high accuracy.

⇒ perform multipole expansion of potential on both the "source" and "sink" sides just once — this can then be reused for all particles in each node

fast multipole method



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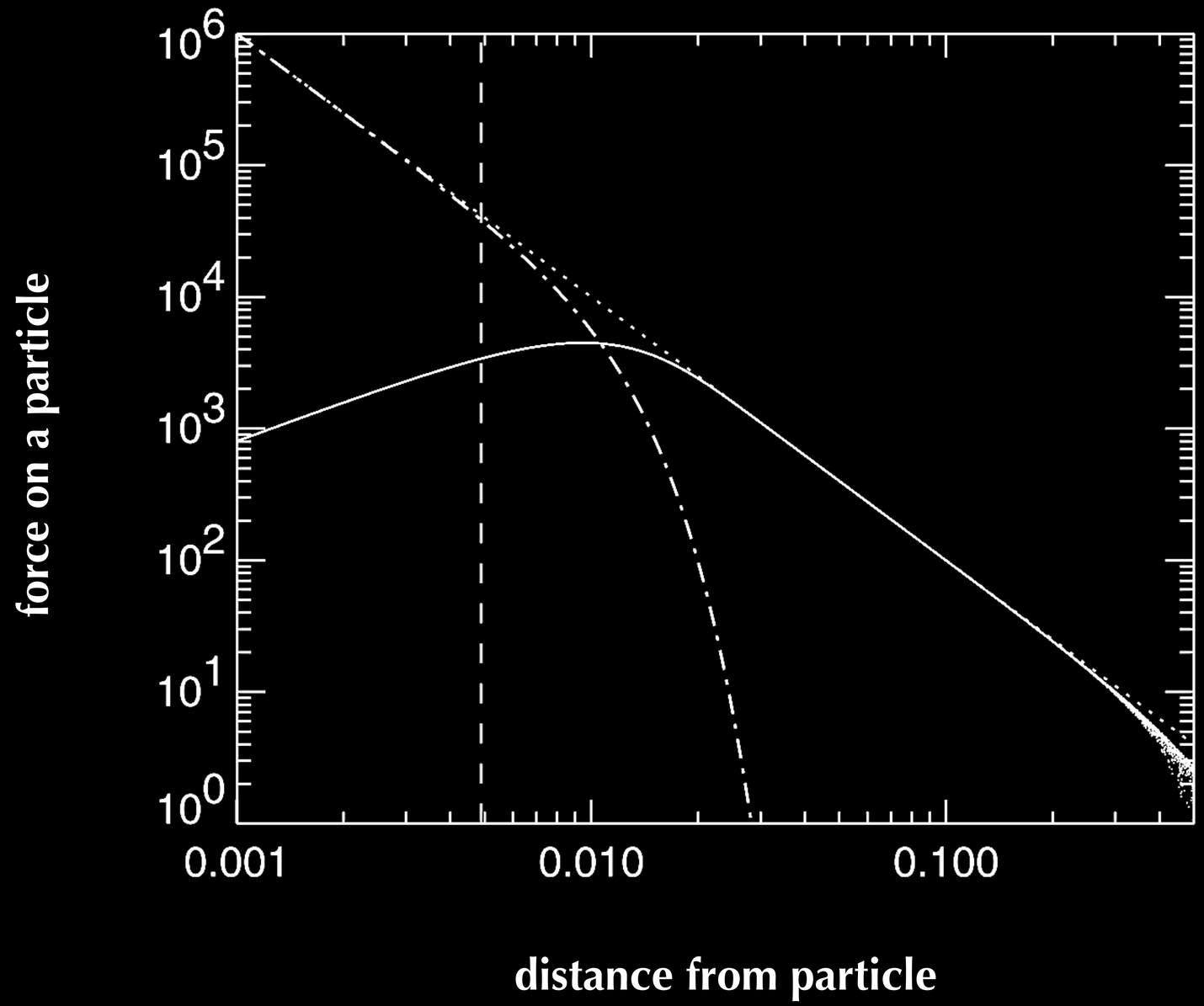
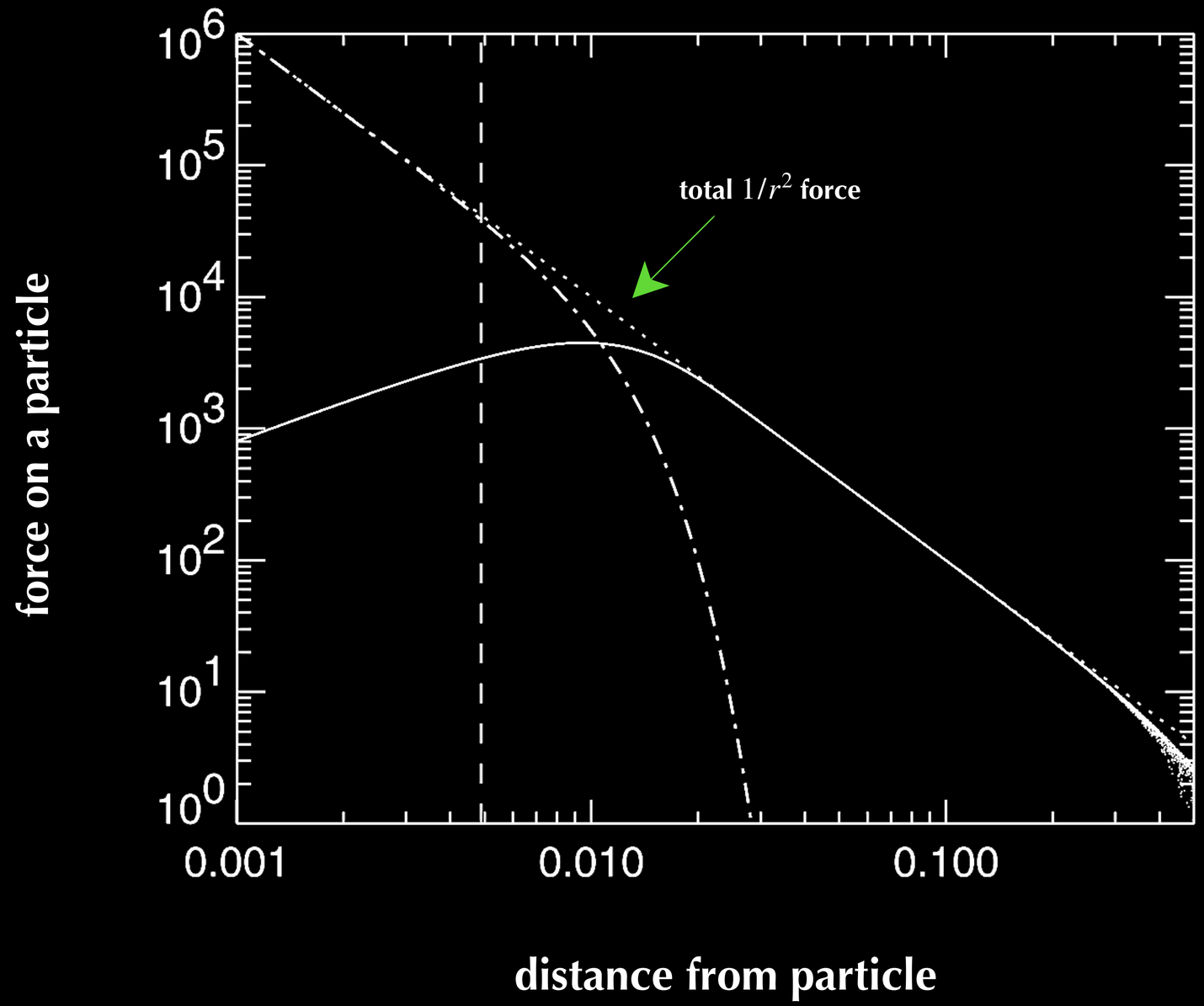
$$g\left(\tilde{\mathbf{x}}_j - \mathbf{x}_i\right) \simeq \sum_{n=0}^{p} \frac{1}{n!} \nabla_{\mathbf{r}}^{(n)} g\left(\mathbf{r}\right) \cdot \left(\mathbf{b}_j - \mathbf{a}_i\right)^{(n)}$$

higher-order multipole expansions ⇒ more accurate forces

$p = 1$ (dipole)
$p = 2$ (quadrupole)
$p = 3$ (octupole)
$p = 4$ (hexadecapole)
$p = 5$ (triakontadipole)



Springel (2005)



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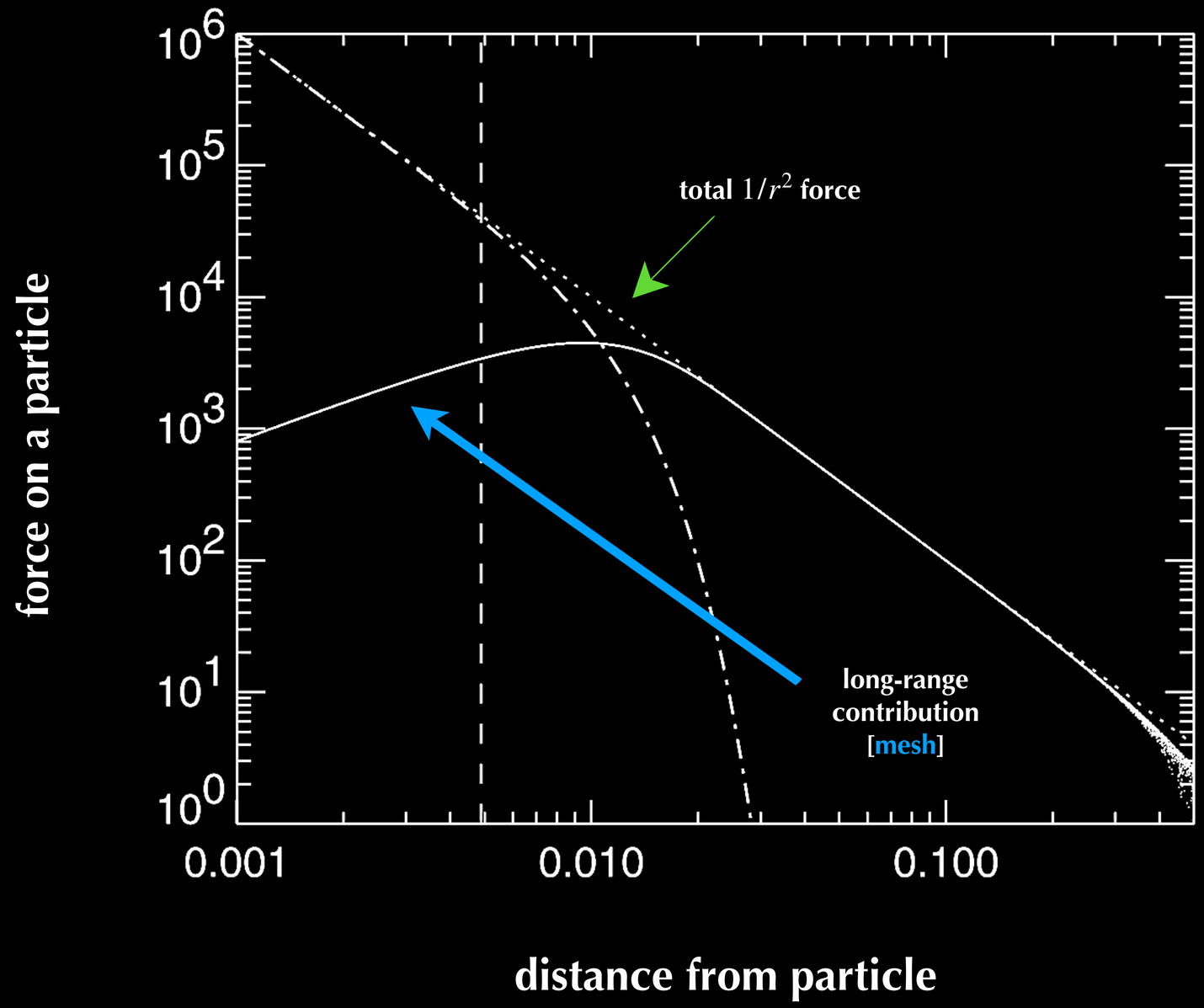

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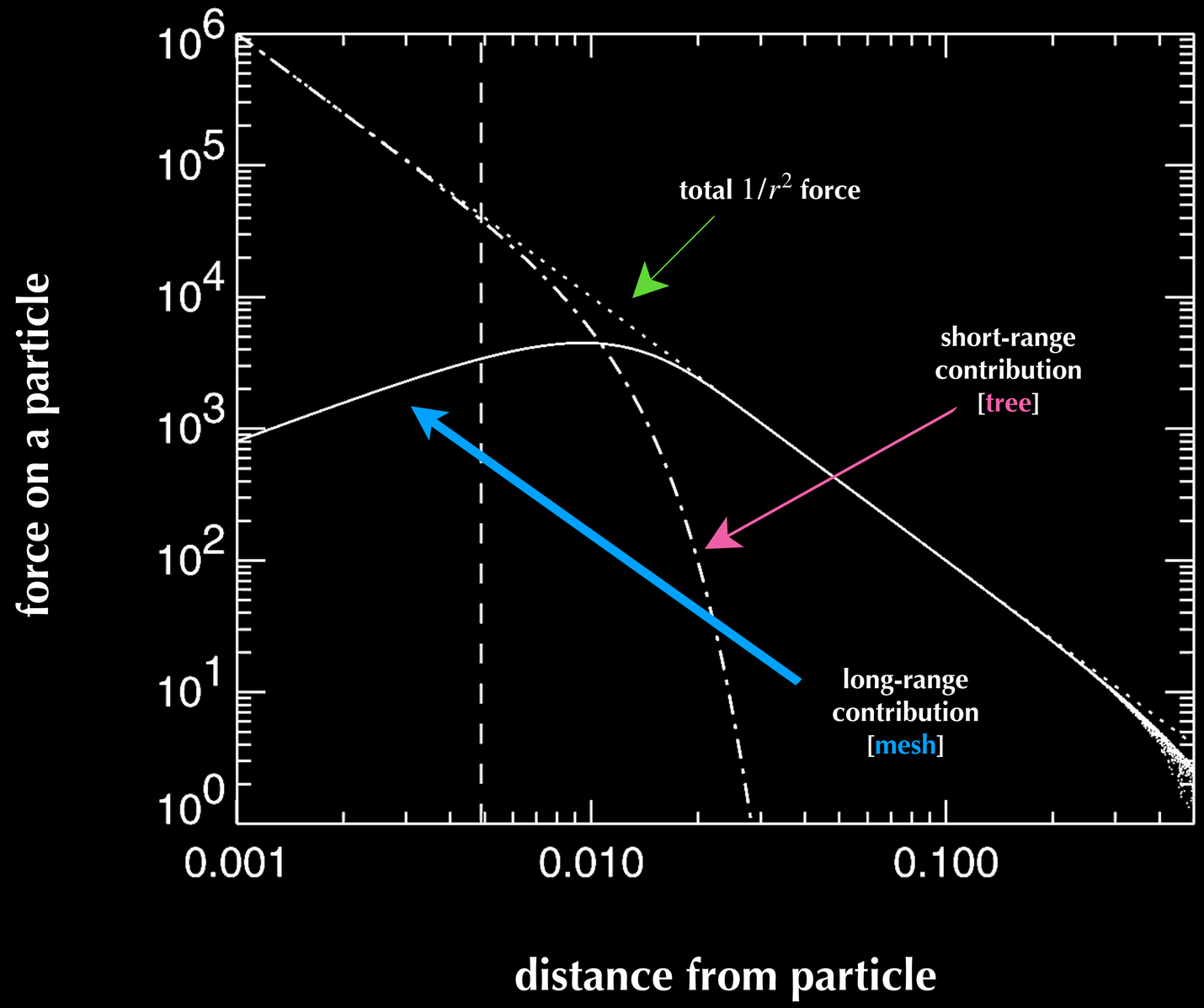

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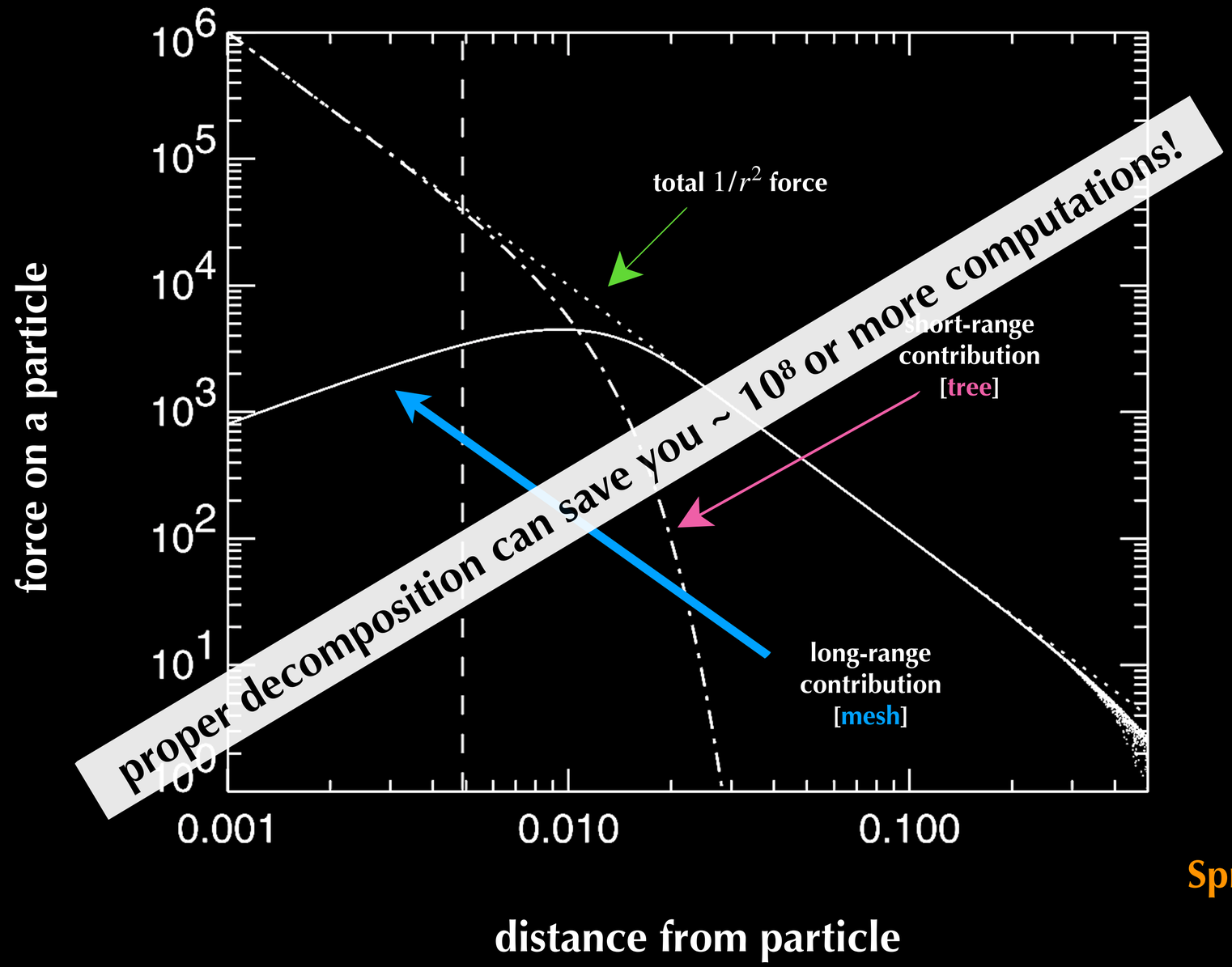

Springel (2005)

basic time integration

once forces on particles have even calculated, we need to propagate these forward in time and update their (1) positions and (2) velocities

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$$\mathbf{x}_j^{n+1} = \mathbf{x}_j^n + \mathbf{v}_j^n \cdot \Delta t$$

$$\mathbf{v}_j^{n+1} = \mathbf{v}_j^n + \mathbf{a}_j^n \cdot \Delta t$$

simplest case: the Euler method

simple

only first-order accurate

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acceleration
[computed from before]

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timestep

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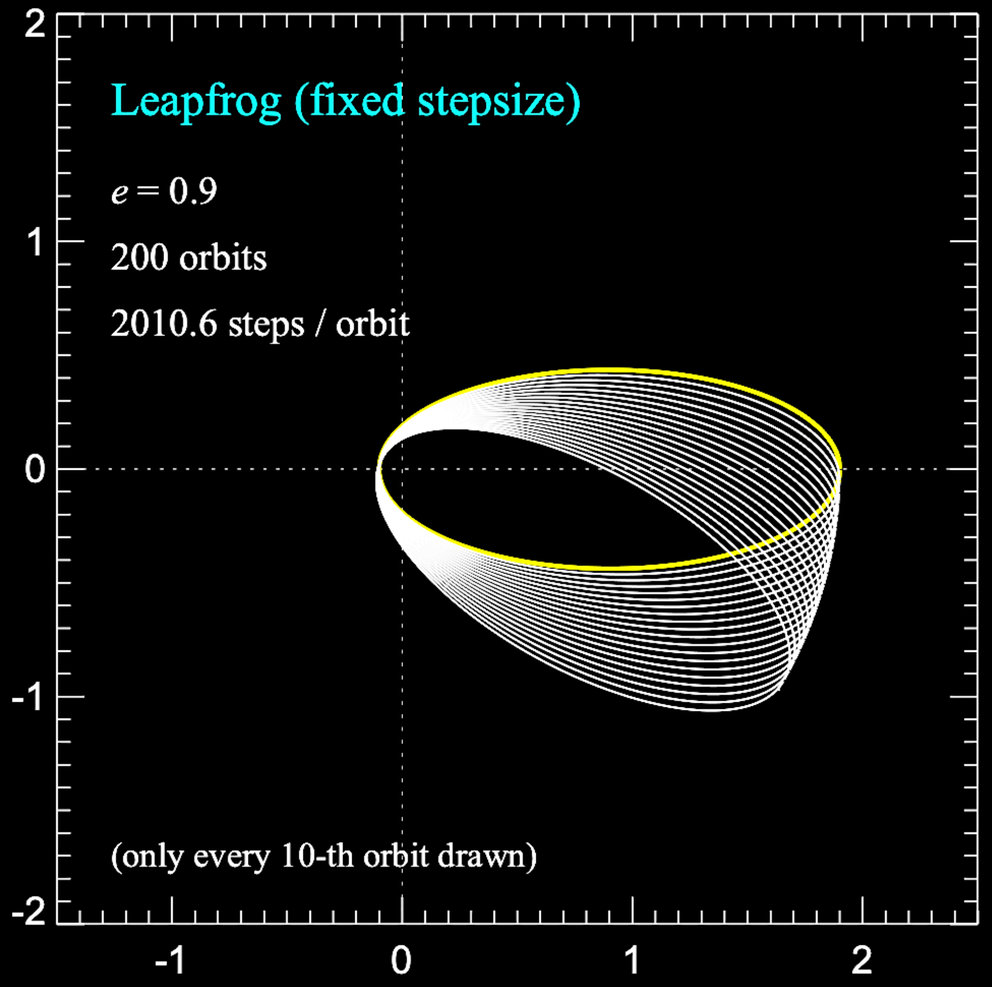
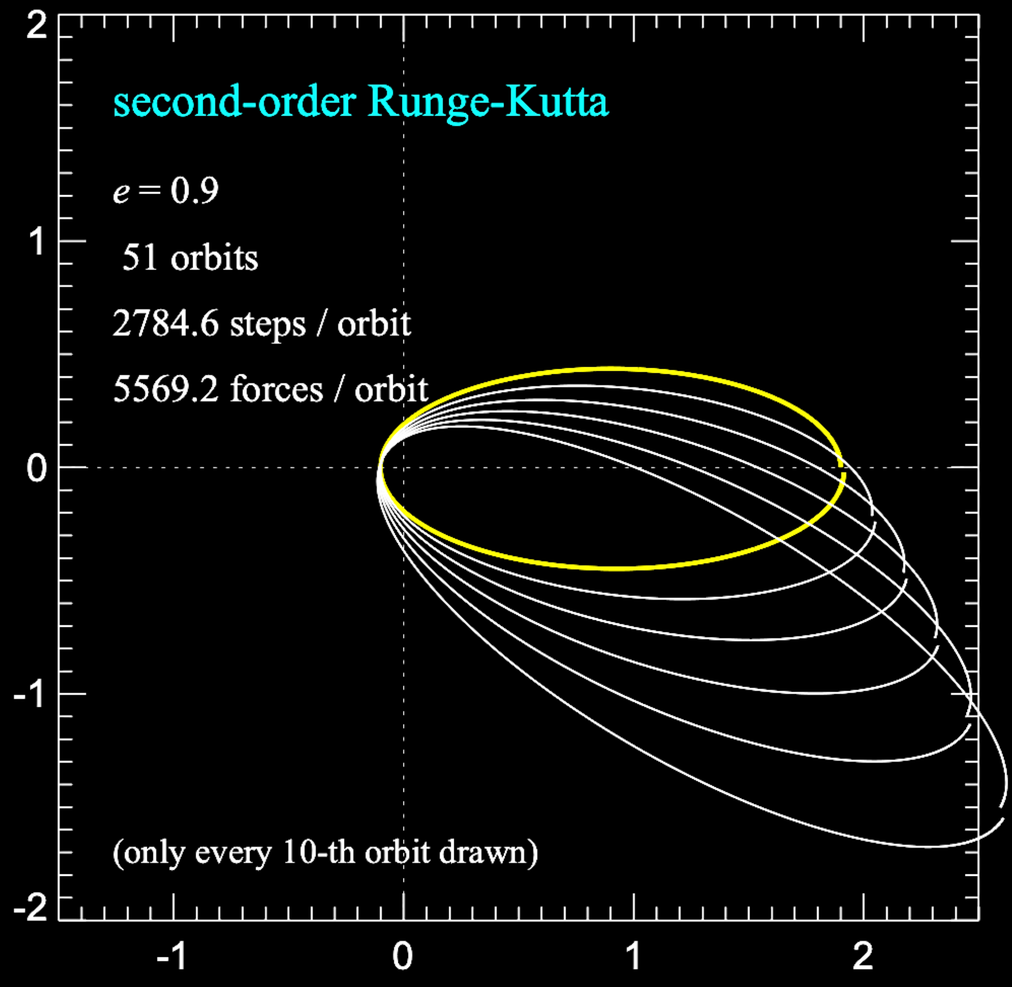
2nd order
"leapfrog" method

much more stable

"symplectic"
[~energy is conserved]





Springel (2005)

choice of timestep

ideally, one would want to choose the size of the timestep, Δt, to be as small as possible

this is impractical from a computational standpoint, but also unnecessary: close-range particle pairs need to be integrated on much shorter timesteps than distant pairs. solution: adopt a hierarchy of timesteps determined by the force acting on the particle

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integration “tolerance” parameter

lecture notes:
https://github.com/sownakbose/PRECISE_Summer_School_Sims

jupyter notebooks:
https://github.com/Shaun-T-Brown/Summer_school