

# Thermal properties of UrQMD box-simulations

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# outline

- 1 motivation
- 2 initialisation of the box
- 3 analysing thermal equilibrium
- 4 thermal properties of ultrarelativistic pion-gas
- 5 shear viscosity
- 6 thermal conductivity
- 7 Summary and Outlook

# short motivation

## why box-calculations?

- final state at CERN, RHIC  
dominated by hadron-interaction  
→ transport coefficients
- transport coefficients as input  
for inmedium models  
(dissipative fluid dynamics)
- low  $\eta/s$  values needed to  
reproduce elliptic flow
- lower bound for  $\eta/s = 1/4\pi$   
suggested (Kovtun Son  
Starinets bound KSS)

# initialisation

use "infinite hadron matter":

- cubic box
- periodic boundary conditions:  
particle leaving at  $\mathbf{r}$  reenters at  $-\mathbf{r}$  with same momentum
- no string-excitations, no 1 to 3 decays:  
destroys detailed-balance
- input to initialise box:  
temperature  $T$  and volume  $V$   
used to calculate number of particles  $N$  and total energy  $E$

# number of particles

first find out number of particles in the system  
 from relativistic kinetic theory: number of particles in a phase space volume

$$dN = f(x, p) \frac{d^3x d^3p}{(\hbar c)^3 (2\pi)^3}$$

use Maxwell-Jüttner distribution function  $f$  in local Lorentz rest frame at high temperatures

Number of particles:

$$N = g_s g_I \frac{V}{(2\pi)^3 (\hbar c)^3} \int_{-\infty}^{+\infty} p^0 e^{-\frac{p^0}{T}} \frac{d^3p}{p^0}$$

$$N = g_s g_I \frac{2 V m^2 T}{(2\pi)^2 (\hbar c)^3} \kappa_2 \left( \frac{m}{T} \right)$$

# energy of particles

Get energy from energy-momentum tensor:

$$T^{\mu\nu} = \int p^\mu p^\nu f \frac{d^3\mathbf{p}}{p^0},$$

energy density is  $T^{00}$  and thus:

$$E = g_s g_I \frac{V}{(2\pi)^3 (\hbar c)^3} \int_{-\infty}^{\infty} p^0 e^{-\frac{p^0}{T}} d^3\mathbf{p}$$

solve analytically:

$$E = g_s g_I \frac{3}{2} \frac{Vm^2 T^2}{\pi^2 (\hbar c)^3} \left( \kappa_2 \left( \frac{m}{T} \right) + \frac{1}{3} \frac{m}{T} \kappa_1 \left( \frac{m}{T} \right) \right)$$

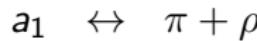
# check thermal equilibrium

Initialize a box with  $\pi$ ,  $\eta$ ,  $\rho$  and  $a_1$  mesons.

Calculate particle numbers and energies at  $T = (80, 100, 110, 120, 130, 140, 150, 160, 170, 180, 200 \text{ and } 220 \text{ MeV})$ .

The  $\eta$ -meson is stable.

The allowed inelastic channels:



# check thermal equilibrium

temperature from thermal pion-distribution:

$$\frac{dN}{d|\mathbf{p}|} = g_{\text{IGS}} \cdot \frac{2V}{(2\pi)^2 \hbar^3} \cdot |\mathbf{p}|^2 \cdot \exp\left(-\frac{\sqrt{m_\pi^2 + |\mathbf{p}|^2}}{T}\right)$$

linearize this equation:

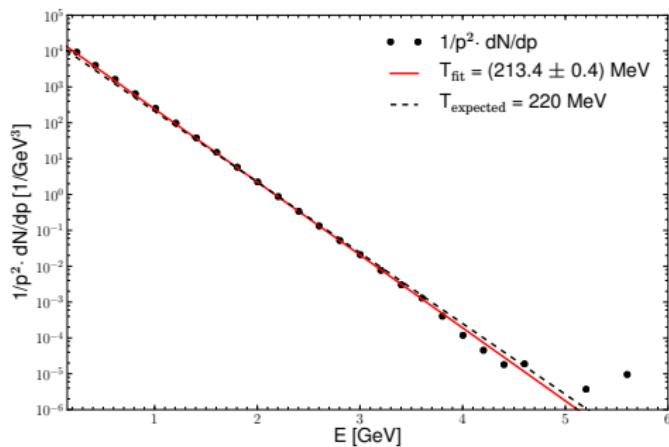
$$\ln\left(\frac{1}{|\mathbf{p}|^2} \cdot \frac{dN}{d|\mathbf{p}|}\right) = A \cdot E + B$$

A: inverse of the temperature and

$$B = \ln\left(\frac{g_{\text{IGS}} 4\pi V}{(2\pi)^3 \hbar^3}\right)$$

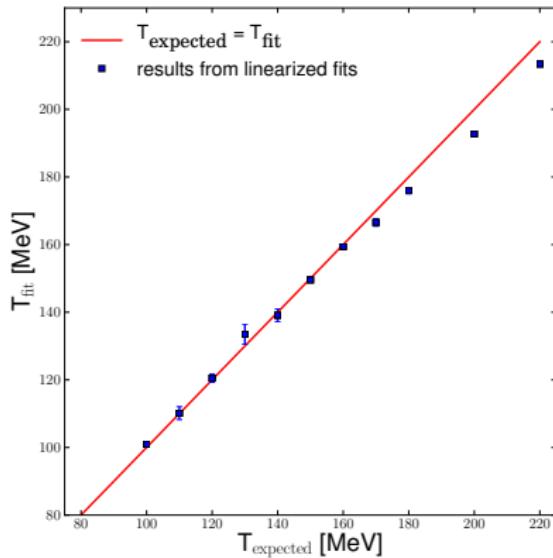
# check thermal equilibrium

extract temperature T from thermal pion distribution



# check thermal equilibrium

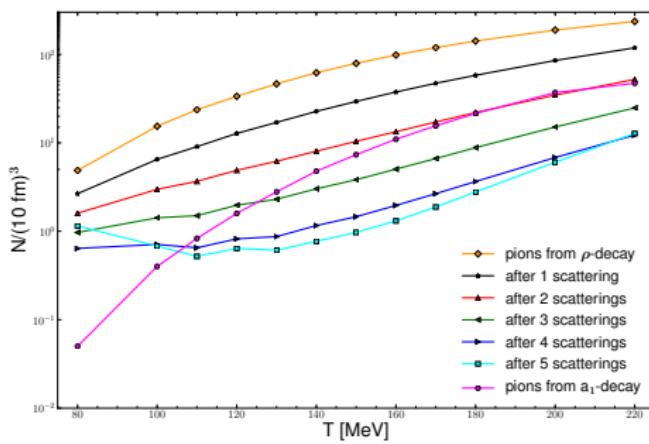
Results for temperature-fits for different temperatures:



Why is the temperature (of the pions) too low for high temperatures?

# check thermal equilibrium

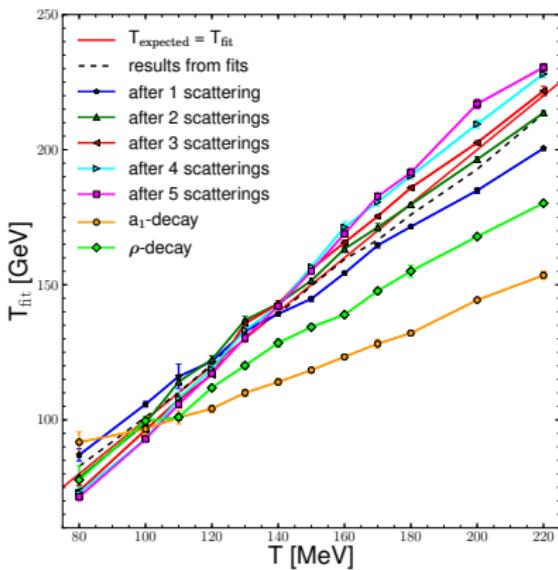
What are the sources of the pions?



- main-pion source:  
 $\rho$ -decay
- $a_1$  decay relevant for  
higher temperatures
- large number of pions  
with  $\geq 5$  scatterings for  
low T:  
 $a_1$  channel starts to play  
role for higher T

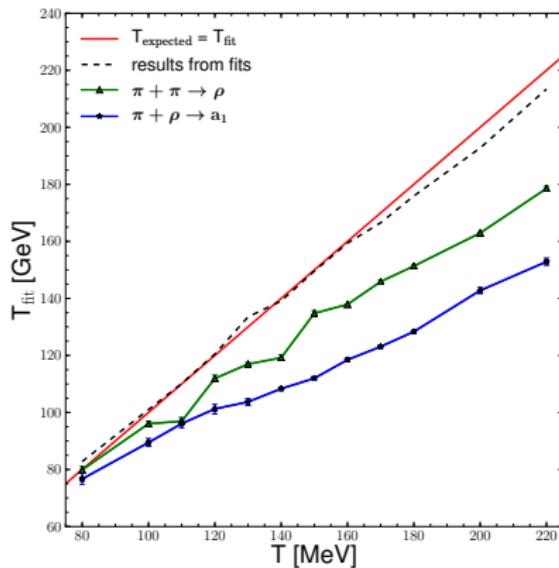
# check thermal equilibrium

temperatures from different sources



→ Pions stemming from  $\rho$  and  $a_1$  decay are colder than medium.  
But:  
Why are pions getting hotter?

# check thermal equilibrium



→ Pions incoming in inelastic scatterings are colder than medium.

# results of first part

- linear fitting itself works good (compared to exponential fitting)
- $a_1$  channel only relevant for high T
- gap between temperature of pions from decay and medium increases with higher overall-T
- additional effect: pions, that form  $\rho$  and  $a_1$ , are colder than medium

# analysis of further thermodynamic quantities

We use temperature T and volume V to calculate:

- energy E
- particle number N

We extract

- the energy density  $\epsilon$
- the isotropic pressure P
- the entropy using Gibbs formula  $s = 1/T(\epsilon + P - \mu_B\rho_B)$ .
- check Gibbs formula for whole box and virtual box inside the whole
- shear viscosity  $\eta$ , viscosity to entropy ratio  $\eta/s$  and thermal conductivity  $\kappa$  and compare to analytic calculations in the ultra-relativistic limit using Green-Kubo formulas.
- extract  $\eta$  (and  $\eta/s$ ) for baryonic medium

# isotropic pressure and entropy

Isotropic pressure from diagonal part of energy-momentum-tensor:

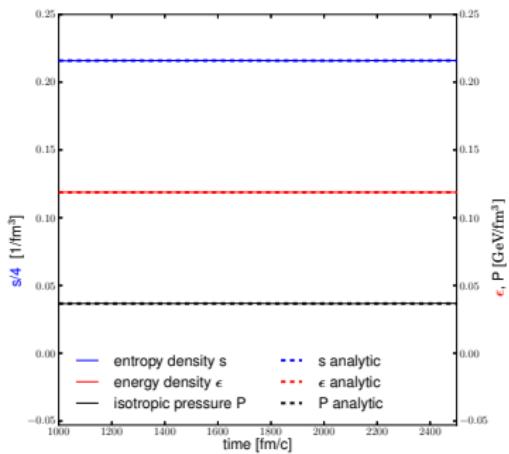
$$P = \frac{1}{3} \int |\mathbf{p}|^2 f \frac{d^3\mathbf{p}}{p^0} = \dots = g_s g_I \frac{2}{(2\pi)^2} \frac{1}{(\hbar c)^3} m^2 T^2 \kappa_2 \left( \frac{m}{T} \right)$$

Entropy:

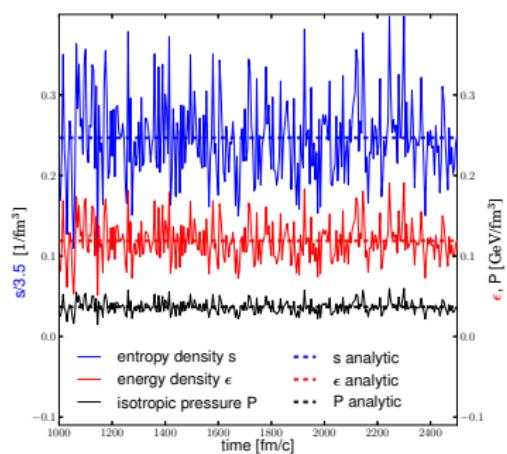
$$\begin{aligned} S &= -4\pi V \int_0^\infty f \left( \ln \left( \frac{(\hbar c)^3}{g_s g_I} f \right) - 1 \right) |\mathbf{p}|^2 d|\mathbf{p}| \\ &= \dots = g_s g_I \frac{V}{2\pi^2 (\hbar c)^3} m^3 \cdot \left( \kappa_1 \left( \frac{m}{T} \right) + 4 \frac{T}{m} \kappa_2 \left( \frac{m}{T} \right) \right) \end{aligned}$$

# fluctuation of the quantities

whole box



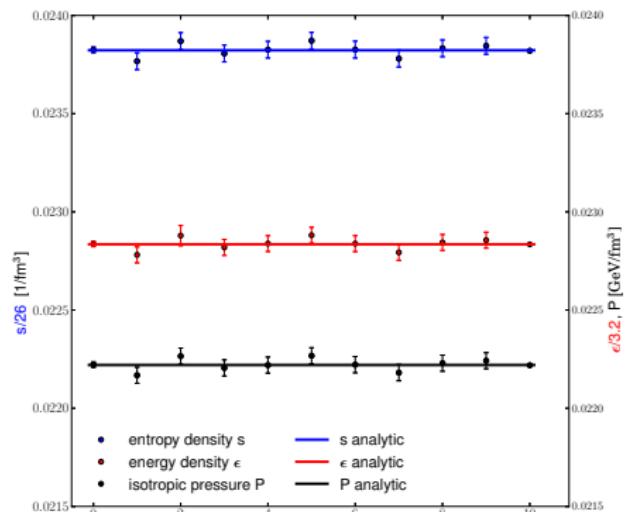
box in center



$T = 180$  MeV

# position of smaller box

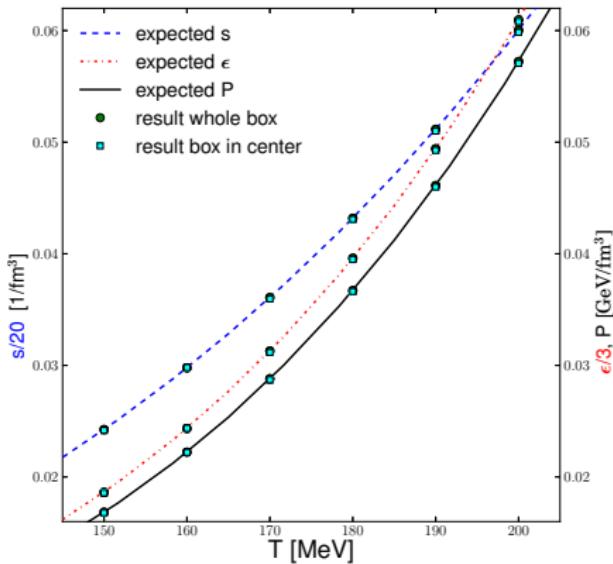
Is it important where to put smaller box?



- 1-8: box in each corner
- 9: box in center
- 0: average over 1-9
- 10: whole box

$T = 160 \text{ MeV}$

# results for different temperatures T



calculation:

$$\epsilon = \frac{1}{V} \sum_{i=1}^{N_{\text{particles}}} p_i^0$$

$$P = \frac{1}{3V} \sum_{i=1}^{N_{\text{particles}}} \frac{|\mathbf{p}_i|^2}{p_i^0}$$

$$s = 1/T \sum_{i=1}^{N_{\text{particles}}} (\epsilon_i + P_i)$$

# $\eta$ : mechanical definition

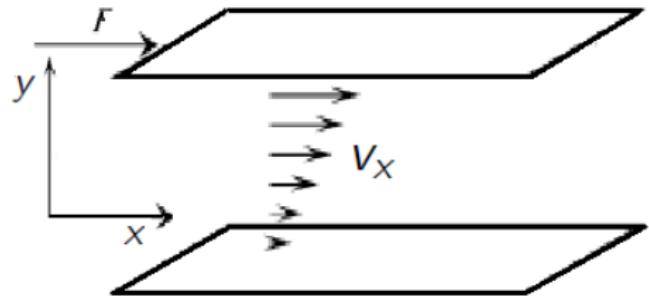
shear force:

→ velocity flow field

→ non-zero  $P^{xy}$

shear viscosity (coefficient)  $\eta$ :

$$P^{xy} = -\eta \frac{\partial v_x}{\partial y}$$



in transport models:

use linear response theory (Green Kubo) to extract  $\eta$ :

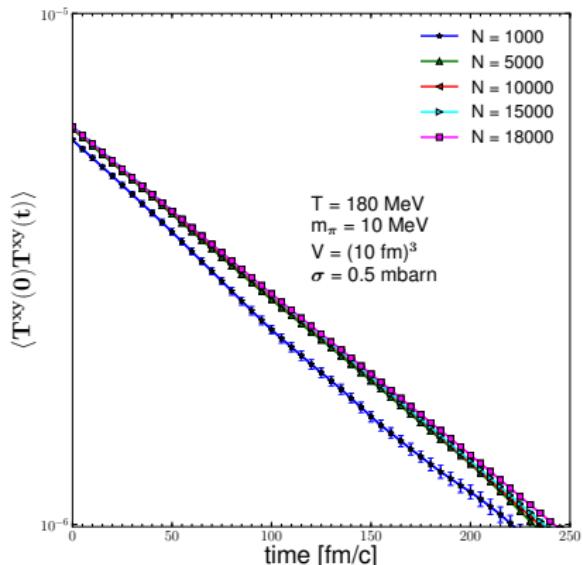
$$\eta = \frac{V}{T} \int_0^{\infty} \langle \pi^{xy}(0) \pi^{xy}(t) \rangle_{\text{eq.}} dt$$

$$\pi^{xy} = T^{xy} = \sum_{i=1}^{N_{\text{particles}}} \frac{p_i^x p_i^y}{p_i^0}$$

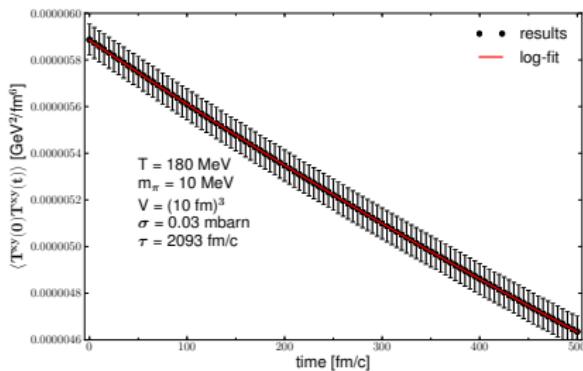
# ensemble average

$$\langle \pi^{xy}(0)\pi^{xy}(t) \rangle_{\text{eq.}} = \frac{1}{N_{\text{events}}} \sum_{i=1}^{N_{\text{events}}} \frac{1}{N} \sum_{i=1}^N T^{xy}(i\Delta t) T^{xy}(i\Delta t + t)$$

- How many timesteps  $N$ ?  
We use 18000
- How many independent box-calculations ? question of storage volume; at least 150  $N_{\text{events}}$



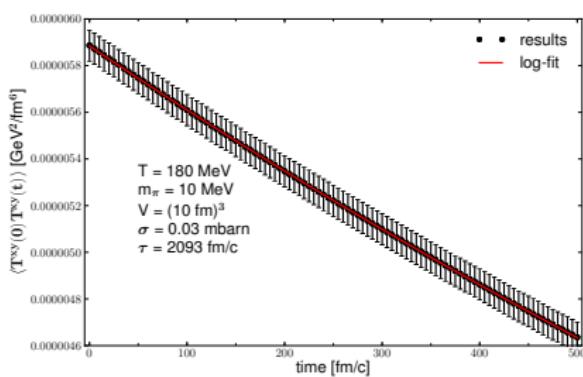
# integrate correlation function



$$\int_0^\infty \langle \pi^{xy}(0)\pi^{xy}(t) \rangle_{\text{eq}} dt$$

How to integrate the correlation function over time?  
→ correlation function decays exponentially

# integrate correlation function



Hence we can write:

$$\begin{aligned}\eta &= \frac{V}{T} \int_0^\infty \langle T^{xy}(0) T^{xy}(t) \rangle_{\text{eq.}} dt \\ &= \frac{V}{T} \int_0^\infty e^{-\frac{t}{\tau}} \cdot \langle T^{xy}(0)^2 \rangle_{\text{eq.}} dt \\ &= \frac{V}{T} \cdot \tau \cdot \langle T^{xy}(0)^2 \rangle_{\text{eq.}}\end{aligned}$$

$\tau$ : relaxation time

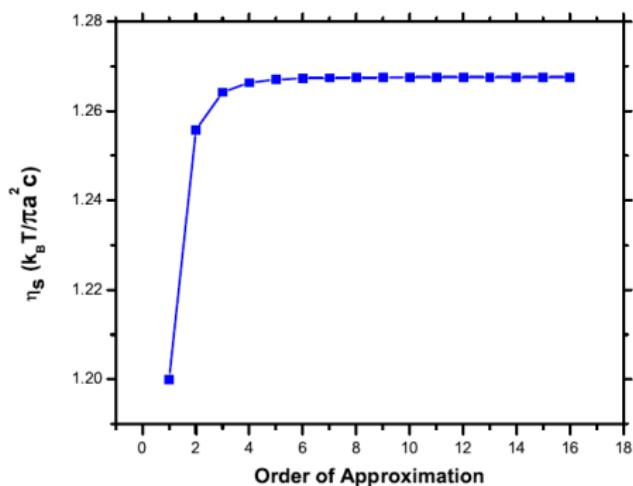
# comparing with analytic results

Now, compare to the results from  
A. Wiranata and M. Prakash,  
arXiv:1203.0281 (2012)  
For a ultra-relativistic hard sphere  
gas one can write:

$$\eta \approx 1.27 \cdot \frac{T}{\sigma}$$

T: temperature

$\sigma$ : total cross section



# ultrarelativistic-limit?

have to satisfy ultra-relativistic and hard-sphere-limit

additional assumptions:

Ultra-relativistic means massless particles and coldness  $\varsigma = m/T = 0$ .  
We try:

- coldness  $\varsigma = m/T \ll 1$
- mass:  $m_\pi$  138 MeV  $\rightarrow$  10 MeV
- temperature:  $T = 180$  MeV

- isotropic cross-section
- one-component gas, binary, elastic scatterings
- hard-sphere approx.:  
const. differential cross-section:  
$$\sigma = a^2/4$$
  
total cross-section:  $\sigma_T = \pi a^2$   
a: radius of sphere

# comparing with Green Kubo

compare Green Kubo

$$\eta = \frac{V}{T} \cdot \tau \cdot \langle T^{xy}(0)^2 \rangle_{\text{eq.}}$$

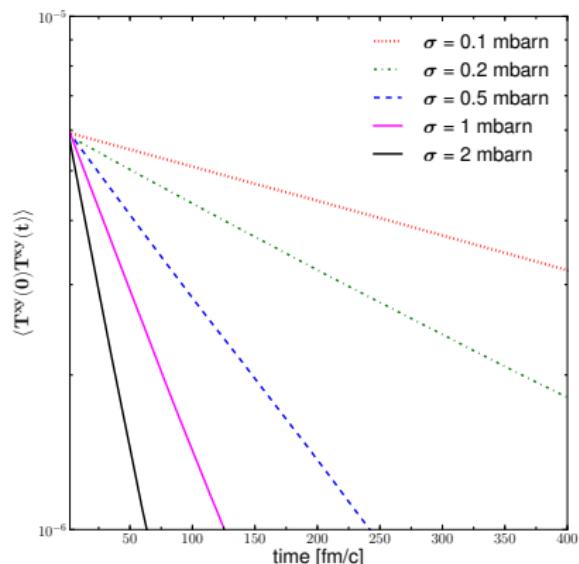
with

$$\eta \approx 1.27 \cdot \frac{T}{\sigma}$$

has  $T$ -,  $\sigma$ -dependence

$\sigma$ -screening:

$\langle T^{xy}(0)^2 \rangle_{\text{eq.}}$  stays the same, but  $\tau$  changes



# $\sigma$ -screening

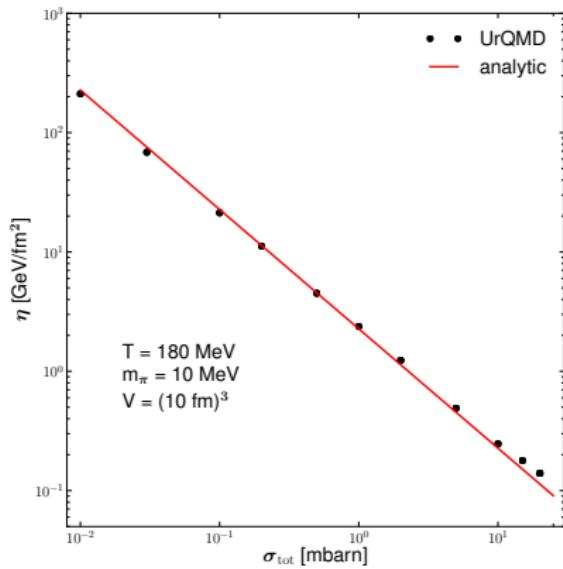
compare Green Kubo

$$\eta = \frac{V}{T} \cdot \tau \cdot \langle T^{xy}(0)^2 \rangle_{\text{eq.}}$$

with

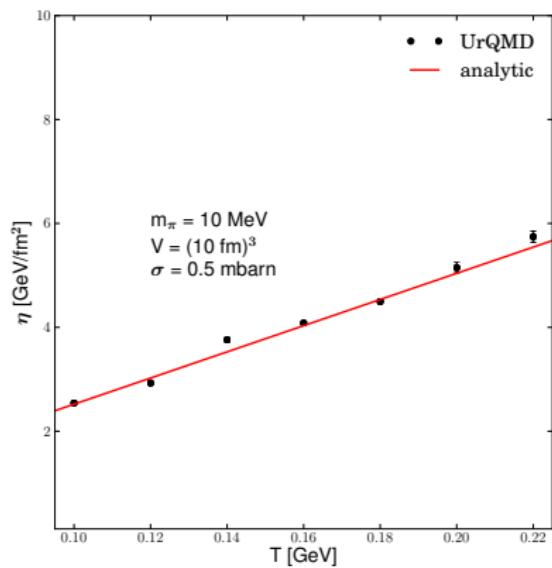
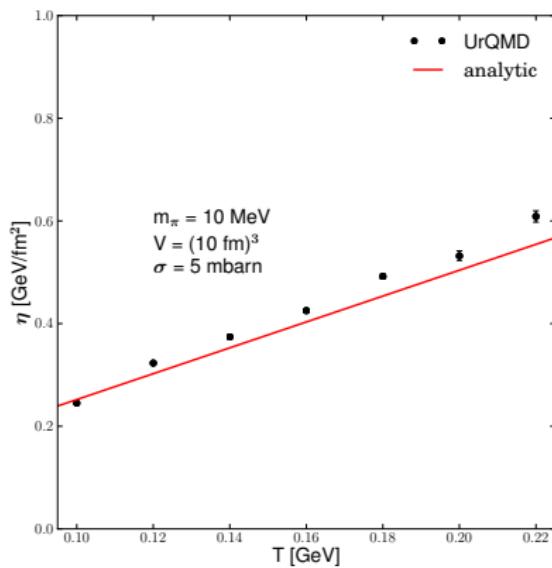
$$\eta \approx 1.27 \cdot \frac{T}{\sigma}$$

here  $\sigma$ -dependence



# temperature screening

$\eta$  vs. temperature T



$\eta/s$ calculate  $\eta/s$  using

compare with analytic:

- viscosity from:

- Green Kubo results
- extracted value for s from

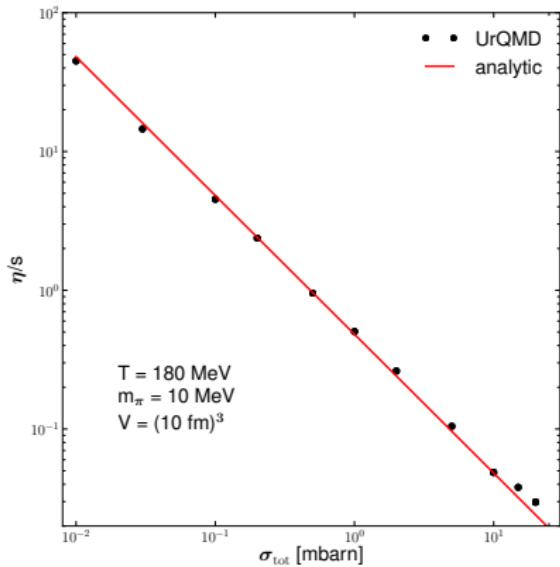
$$s = 1/T \sum_{i=1}^{N_{\text{particles}}} (\epsilon_i + P_i)$$

- entropy from:

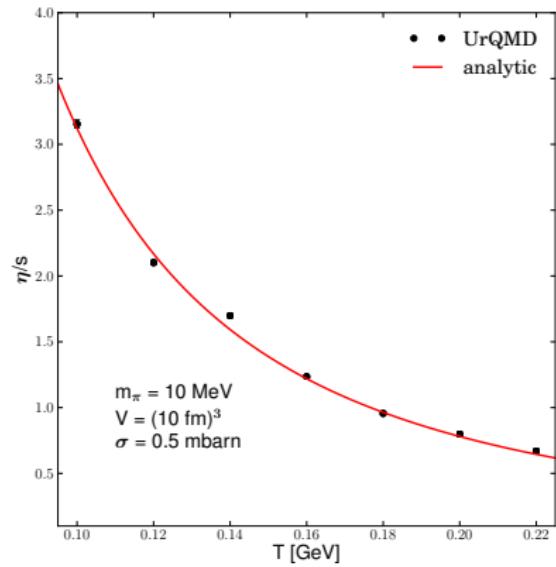
$$s = g_S g_I \frac{1}{2\pi^2 \hbar^3} m_i^3 \cdot \left( \kappa_1 \left( \frac{m}{T} \right) + 4 \frac{kT}{m_i c^2} \kappa_2 \left( \frac{m}{T} \right) \right)$$

# $\eta/s$ results

$\eta/s$  vs. cross-section  $\sigma$



$\eta/s$  vs. temperature  $T$



# $\eta$ for box including baryons

different setting:

box with nucleons,  $\pi$ -mesons and  $\Delta_{1232}$ -resonances.

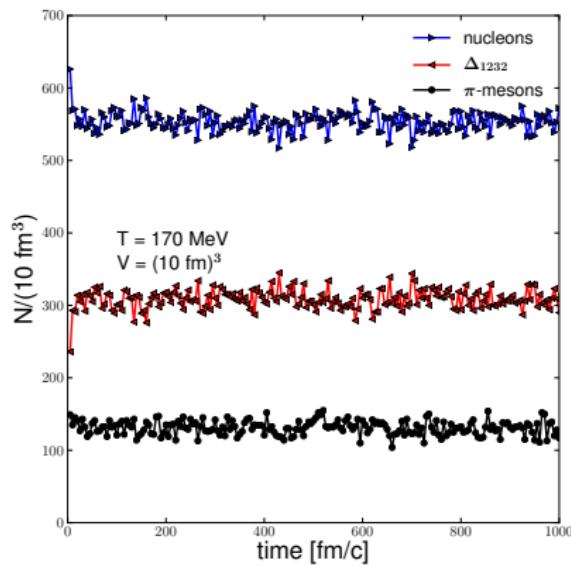
$$\pi + n \leftrightarrow \Delta_{1232}$$

Motivation:

since  $\eta \sim \frac{|\vec{p}|}{\sigma}$ , one might see where  $N_{pions} = N_{nucleons}$

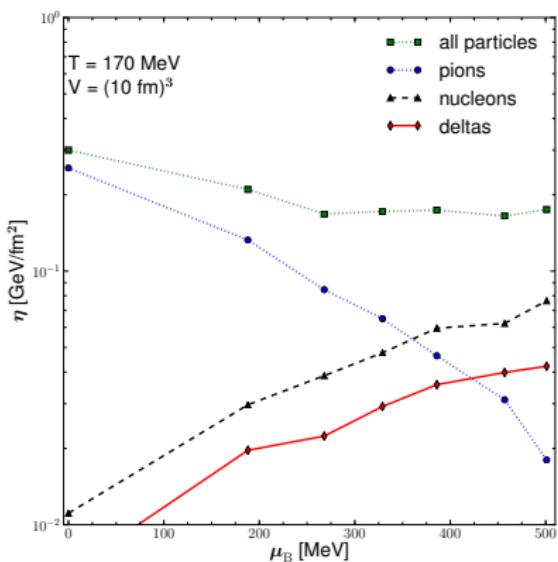
→ change baryon number by introducing baryo-chemical potential  $\mu_B$

# thermalization



- chemical-equilibrium realized very fast
- we assume thermal-equilibrium is realized after 1000 fm/c

# results $\eta$



- note:  
use extracted temperature  $T$
- $\eta$  falls and saturates
- to do: extract  $s$  for  $\eta/s$   
difficulty:  
get real  $\mu_B$

# thermal conductivity $\kappa$

isotropic medium: heat flux  $\mathbf{q}$ , thermal conductivity  $\kappa$ :

$$\mathbf{q} = -\kappa \nabla T$$

$\mathbf{q}$ : heat flowing per second and per unit area

thermal conductivity  $\kappa$  (Green Kubo):

$$\kappa = \frac{V}{T^2} \int_0^\infty dt \langle q^\mu(0) q^\mu(t) \rangle_{\text{eq.}}$$

relativistic heat flow  $q^\mu$ :

$$q^\mu = (u_\nu T^{\nu\sigma} - h N^\sigma) h_\sigma^\mu.$$

→ difference of energy flow and flow of enthalpy  $h$  carried by the particles

$h = (en + p)/n$ : heat function per particle

$u^\mu$ : hydrodynamic velocity

$h^{\mu\nu} = g^{\mu\nu} - u^\mu u^\nu$ : projector → gives part  $\perp u^\mu$

# heat flow

heat flow depends strongly on decomposition

Eckart's definition:

$$u_E^\mu = \frac{N^\mu}{\sqrt{N^\nu N_\nu}}$$

$$\rightarrow h^{\mu\nu} N_\nu = 0$$

$$q_E^\mu = u_\nu T^{\nu\sigma} h_\sigma^\mu.$$

Landau and Lifshitz's definition:

$$u_L^\mu = \frac{T^{\mu\nu} u_\nu}{\sqrt{u_\rho T^{\rho\sigma} T^{\sigma\tau} u_\tau}}$$

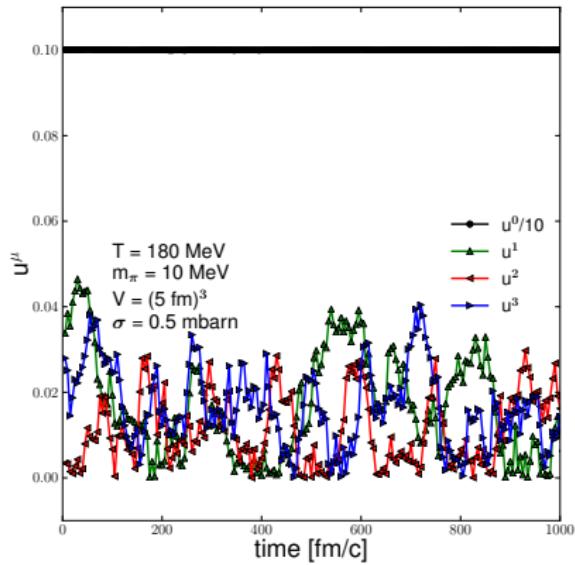
$$\rightarrow h^{\mu\nu} T_{\nu\sigma} u^\sigma = 0$$

$$q_L^\mu = -h N^\sigma h_\sigma^\mu.$$

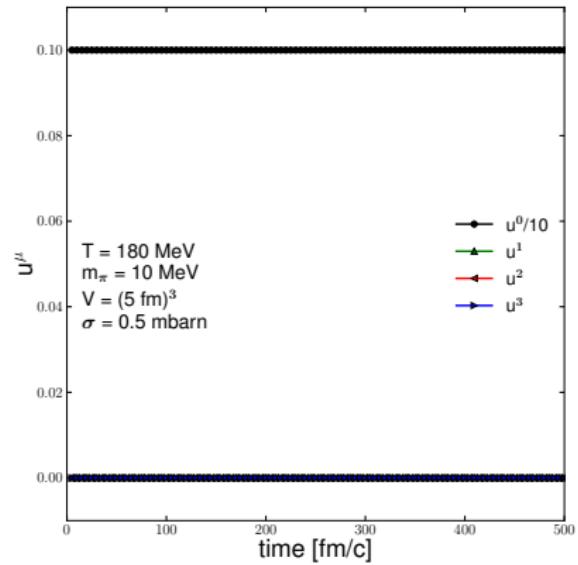
# heat flow

In which local Lorentz rest frame ( $u^\mu = (1, 0, 0, 0)^T$ ) are we?

Eckart:



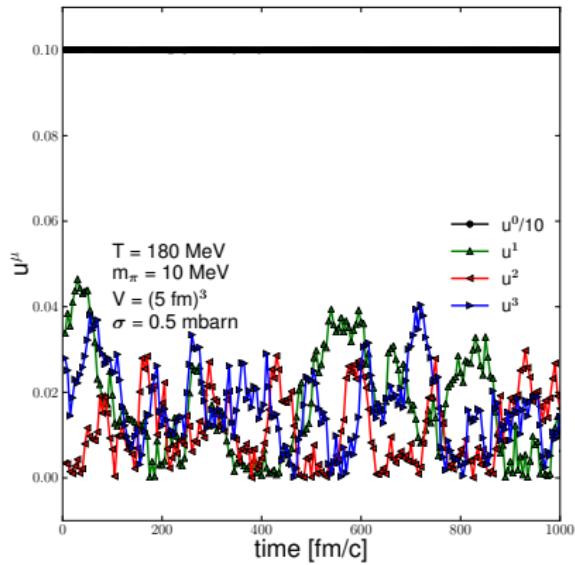
Landau Lifshitz:



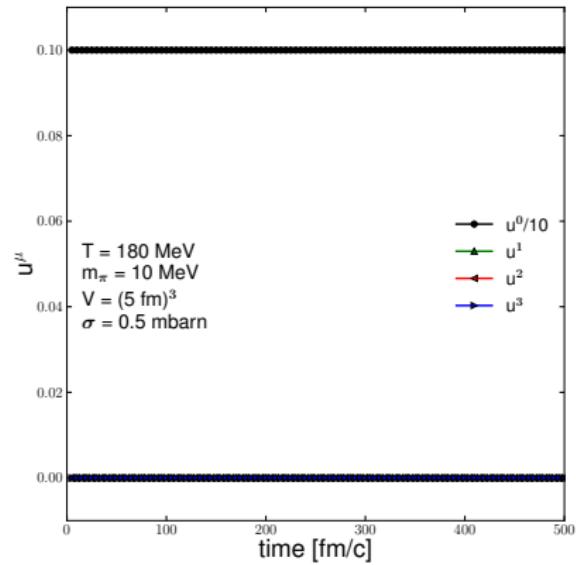
# heat flow

In which local Lorentz rest frame ( $u^\mu = (1, 0, 0, 0)^T$ ) are we?

Eckart:



Landau Lifshitz:



# result heat flow and thermal conductivity

This means for heat flow:

$$q^\mu = -hN^i$$

$N^i$ : flux of particle number per unit time and unit area in i-th spacial direction:

$$N^i = \int p^i f \frac{d^3\mathbf{p}}{p^0}$$

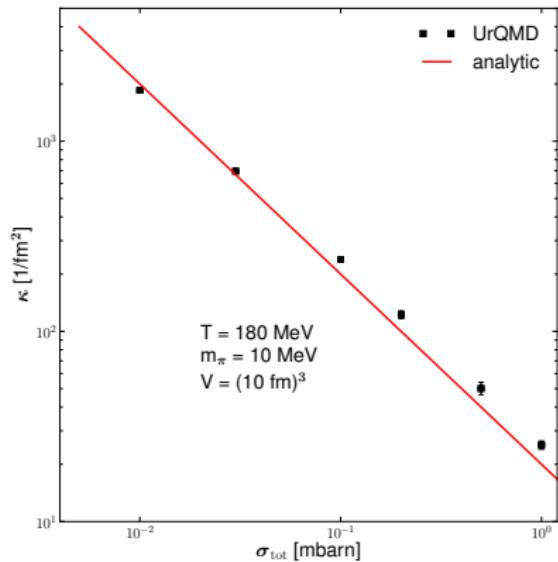
for UrQMD-calculations:

$$N^i = \frac{1}{V} \sum_{i=1}^{N_{particles}} \frac{p^i}{p^0} \quad \rightarrow \quad \kappa = \frac{V}{3T^2} \int_0^\infty \langle h\mathbf{N}(0) \cdot h\mathbf{N}(t) \rangle_0 dt$$

# result thermal conductivity

compare Green Kubo with  
ultra-relativistic hard sphere  
approximation in first order from  
Carlo Cercignani and Gilberto  
Medeiros Kremer (Relativistic  
Boltzmann Equation):

$$\kappa \approx \frac{2}{\sigma} \left( 1 + \left( \frac{m}{T} \right)^2 + \dots \right)$$



# summary and outlook

- extracted thermal properties like pressure  $P$  and entropy  $s$
- extracted  $\eta$  and  $\eta/s$  using Green Kubo:  
successful T- and  $\sigma$ -screening
- $\eta$  for baryonic-medium:  
 $\mu_B$ -screening
- extracted  $\kappa$  using Green Kubo:  
successful  $\sigma$ -screening
- to do:
  - try  $\kappa$  for Eckart decomposition
  - extract  $\mu_B \rightarrow \eta/s$  from baryonic-medium

