Transport Model Evaluation Project (TMEP): Status and Perspectives

Hermann Wolter
University of Munich, ORIGINS Excellence Cluster

NUSYM2024, GANIL, Caen, France, Sep. 9-13, 2024

On behalf of the Transport Model Evaluation Project (TMEP) Collaboration

Progress in Particle and Nuclear Physics 125 (2022) 103962

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

Review

Transport model comparison studies of intermediate-energy heavy-ion collisions

Hermann Wolter [1,*], Maria Colonna [2], Dan Cozma [3], Pawel Danielewicz [4,5], Che Ming Ko [6], Rohit Kumar [4], Akira Ono [7], ManYee Betty Tsang [4,5], Jun Xu [8,9], Ying-Xun Zhang [10,11], Elena Bratkovskaya [12,13], Zhao-Qing Feng [14], Theodoros Gaitanos [15], Arnaud Le Fèvre [12], Natsumi Ikeno [16], Youngman Kim [17], Swagata Mallik [18], Paolo Napolitani [19], Dmytro Oliinychenko [20], Tatsuhiko Ogawa [21], Massimo Papa [2], Jun Su [22], Rui Wang [9,23], Yong-Jia Wang [24], Janus Weil [25], Feng-Shou Zhang [26,27], Guo-Qiang Zhang [9], Zhen Zhang [22], Joerg Aichelin [28], Wolfgang Cassing [25], Lie-Wen Chen [29], Hui-Gan Cheng [14], Hannah Elfner [12,13,20], K. Gallmeister [25], Christoph Hartnack [28], Shintaro Hashimoto [21], Sangyong Jeon [30], Kyungil Kim [17], Myungkuk Kim [31], Bao-An Li [32], Chang-Hwan Lee [33], Qing-Feng Li [24,34], Zhu-Xia Li [10], Ulrich Mosel [25], Yasushi Nara [35], Koji Niita [36], Akira Ohnishi [37], Tatsuhiko Sato [21], Taesoo Song [12], Agnieszka Sorensen [38,39], Ning Wang [11,40], Wen-Jie Xie [41], (TMEP collaboration)

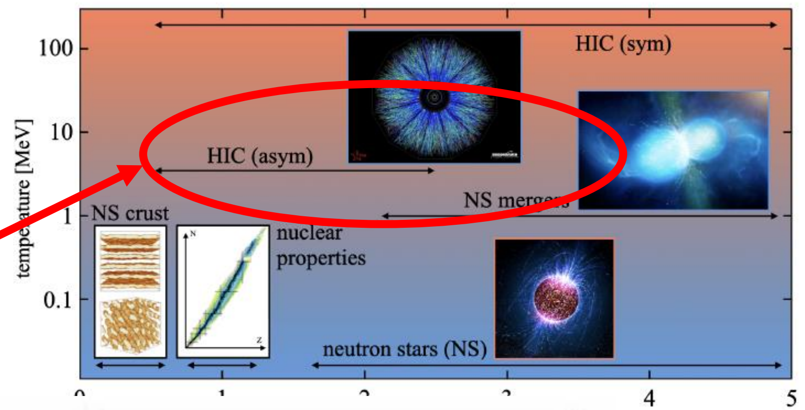
Outline:

- Motivation: Increase impact of HIC studies on determination of EOS
- TMEP strategy: Comparison of transport codes under controlled conditions, similar input -> similar output(?)
- box calculations: test individual ingredients, comparison to exact results,
- HIC: open systems, much less agreement, explanations, but no solid error estimates
- Intermediate conclusions: lessons learned and desirables for more robust conclusions
- Uncertainty quantification: Bayesian inference with many codes, BMA (Bayesian model averaging)
- Alternative: collaboration to construct modular common code

Motivation: Increase impact of HIC in EOS studies

Importance of intermediate-energy heavy-ion collisions for the exloration of equation-of-state (EOS)

→ filling the gap between information from nuclear structure ($\rho \leq \rho_0$) and neutron star observations ($\rho \geq 2.5\ \rho_0$)

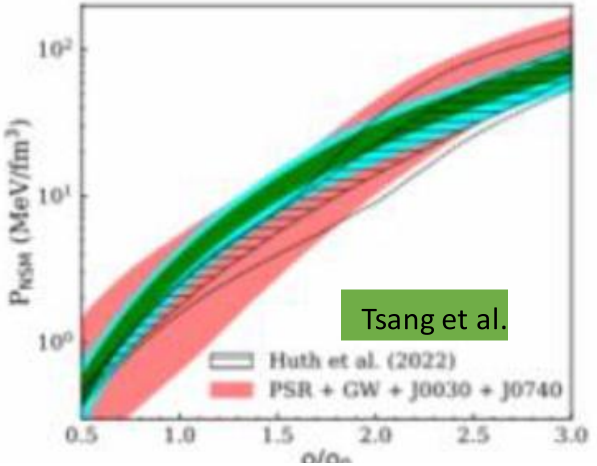


-> can make a contribution to constrain EOS

-> only astrophysics

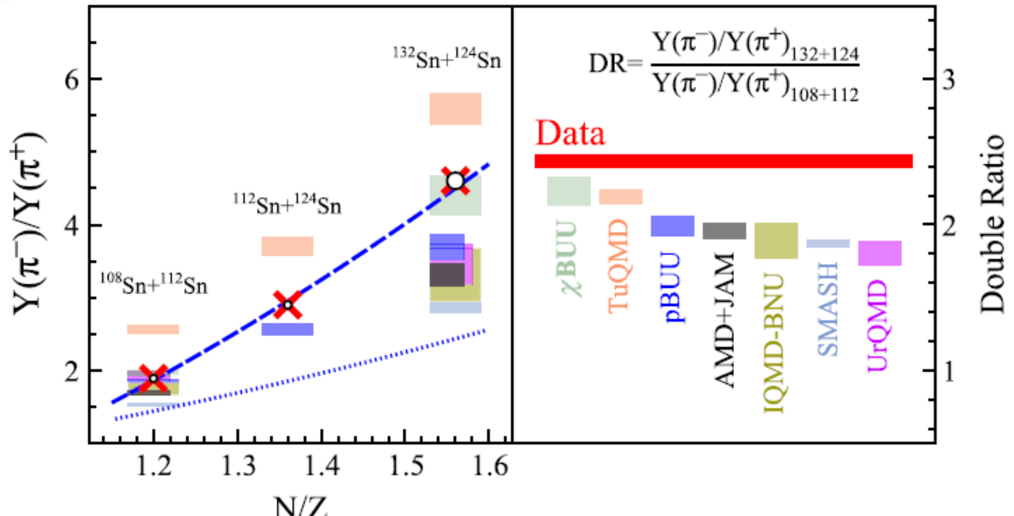
-> xEFT, Astro and HICs (Huth, et al., Nature 602 (22)

-> structure, HICs and Astro (C.Y.Tsang, et al.,Nat.Astro 8 (24)



model dependence of HIC results:

SπRIT data, Sn+Sn, 270 MeV/A,
Jhang, et al., PLB 813 (21)
predictions: best physics model of each code



large spread of results
sensitivity to symmetry energy (size of boxes) relatively small

Transport theory: kinetic equation Boltzmann-Uehling-Uhlenbeck (BUU)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{m}\vec{\nabla}^{(r)} f - (\vec{\nabla}^{(r)} U(r,p)\, \vec{\nabla}^{(p)} + \vec{\nabla}^{(p)} U(r,p)\, \vec{\nabla}^{(r)})\, f(\vec{r},\vec{p};t) = I_{coll} \quad + \delta I_{fluc}$$

$$I_{coll} = \int d\vec{p}_2 d\vec{p}_{1'} d\vec{p}_{2'}\, v_{21}\, \sigma_{12}^{in-med}(\Omega)\, (2\pi)^3 \delta(p_1 + p_2 - p_{1'} - p_{2'}) \left[f_{1'} f_{2'} \bar{f}_1 \bar{f}_2 - f_1 f_2 \bar{f}_{1'} \bar{f}_{2'} \right]$$

Physical model:
mean field->EOS,
in-medium xsec
inelastic collisions

$\bar{f}_i := (1 - f_i)$ Pauli blocking factors,

$I_{coll} \rightarrow I_{el}\,(NN \leftrightarrow NN) + I_{inel}\,(NN \leftrightarrow N\Delta) + I_{decay}\,(\Delta \leftrightarrow N\pi)$

Two main reasons of model dependence: **1) fluctuations, 2) simulation strategies**

1) Two families, depending on representation of phase space density $f(\vec{r},\vec{p};t)$

BUU phase space density represented by test particles (TP) $f(\vec{r},\vec{p};t) = \sum_{TP\ i} \delta(\vec{r} - \vec{r}_i(t))\, \tilde{\delta}(\vec{p} - \vec{p}_i(t))$,
deterministic and exact for #TP$\rightarrow\infty$;
introduce fluctuations explicitely, Boltzmann-Langevin, add term δI_{fluc}

QMD product of wave packets in coordinate space $f(\vec{r},\vec{p};t) = \left(\frac{\hbar}{\sqrt{L}}\right)^3 \sum_i \exp\left[-\frac{(\vec{r} - \vec{R}_i(t))^2}{2L}\right] \delta(\vec{p} - \vec{P}_i(t))$
fluctuations on classical level by ansatz, fluctuations parametrized by width parameter L, „events“

-> Fluctuations influence many aspects of simulation

Transport theory: kinetic equation Boltzmann-Uehling-Uhlenbeck (BUU)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{m}\vec{\nabla}^{(r)} f - (\vec{\nabla}^{(r)} U(r,p)\, \vec{\nabla}^{(p)} + \vec{\nabla}^{(p)} U(r,p)\, \vec{\nabla}^{(r)})\, f(\vec{r},\vec{p};t) = I_{coll}$$

$$I_{coll} = \int d\vec{p}_2 d\vec{p}_{1'} d\vec{p}_{2'}\, v_{21}\, \sigma_{12}^{in-med}(\Omega)\, (2\pi)^3 \delta(p_1 + p_2 - p_{1'} - p_{2'}) \left[f_{1'} f_{2'} \bar{f}_1 \bar{f}_2 - f_1 f_2 \bar{f}_{1'} \bar{f}_{2'} \right]$$

$\bar{f}_i := (1 - f_i)$ Pauli blocking factors,

Physical model:
mean field->EOS,
in-medium xsec
inelastic collisions

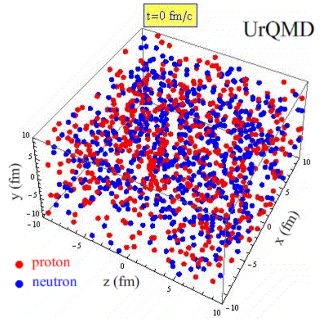
Two main reasons of model dependence: **1) fluctuations, 2) simulation strategies**

2) Transport equation solved by simulations, involves strategies
mf dynamics: - Hamiltonan equations-of-motion (for TP or nucleons)
finite-size TP, use of lattice Hamiltonian,
non-linear density functionals $\propto \rho^{\sigma}$, often approximated in QMD

collision term: - stochastic two-body collisions
geometric coll Kriterien $d < \sqrt{\sigma(\sqrt{s})/\pi}$ $\leftrightarrow$ local thermal equilibrium
blocking: need for averaging, coarse graining, surface

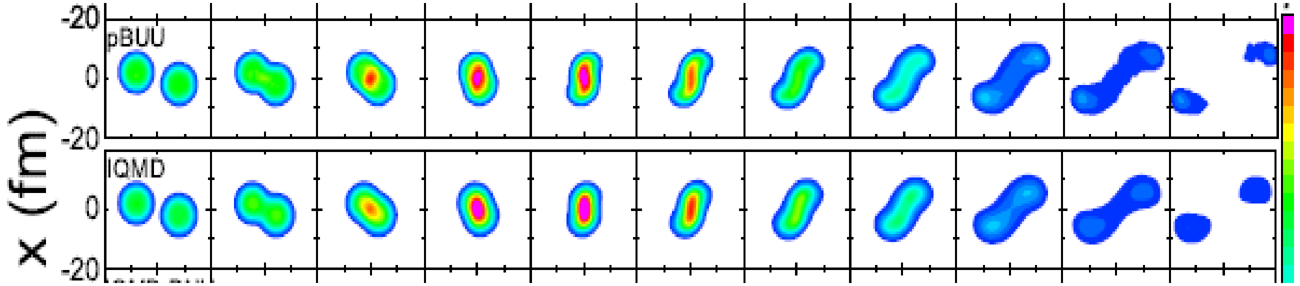
TMEP: compare different transport models und controlled conditions,
same physical model and similar calculational parameters -> similar results??

two modes of comparisons:

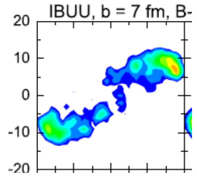


1. box calculations, periodic boundary conditions, simulates infinite nuclear matter,
   study individually different part of physical model,
   compare to exact limits

2, full heavy-ion collisions (HICs),
   compare codes between each other ,
   convergence or amount of disagreement



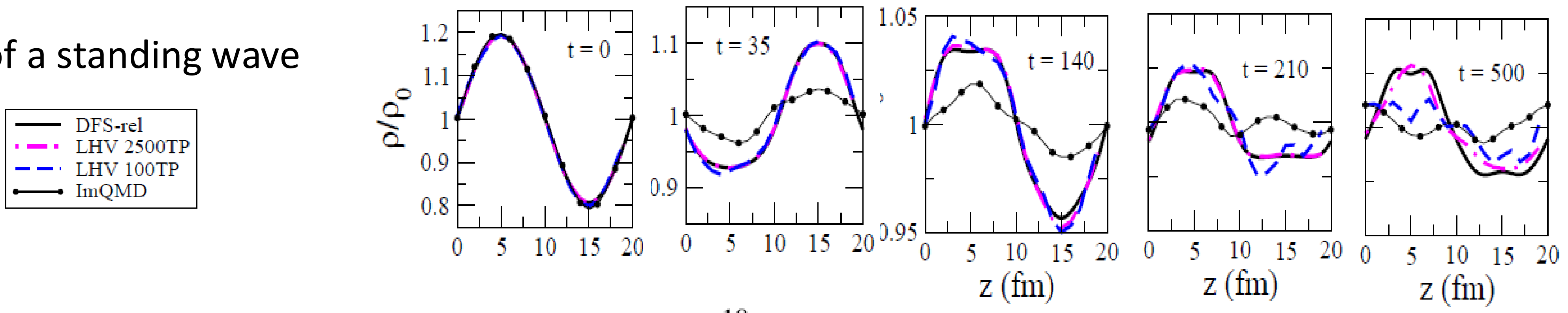
BUU
QMD



QMD event

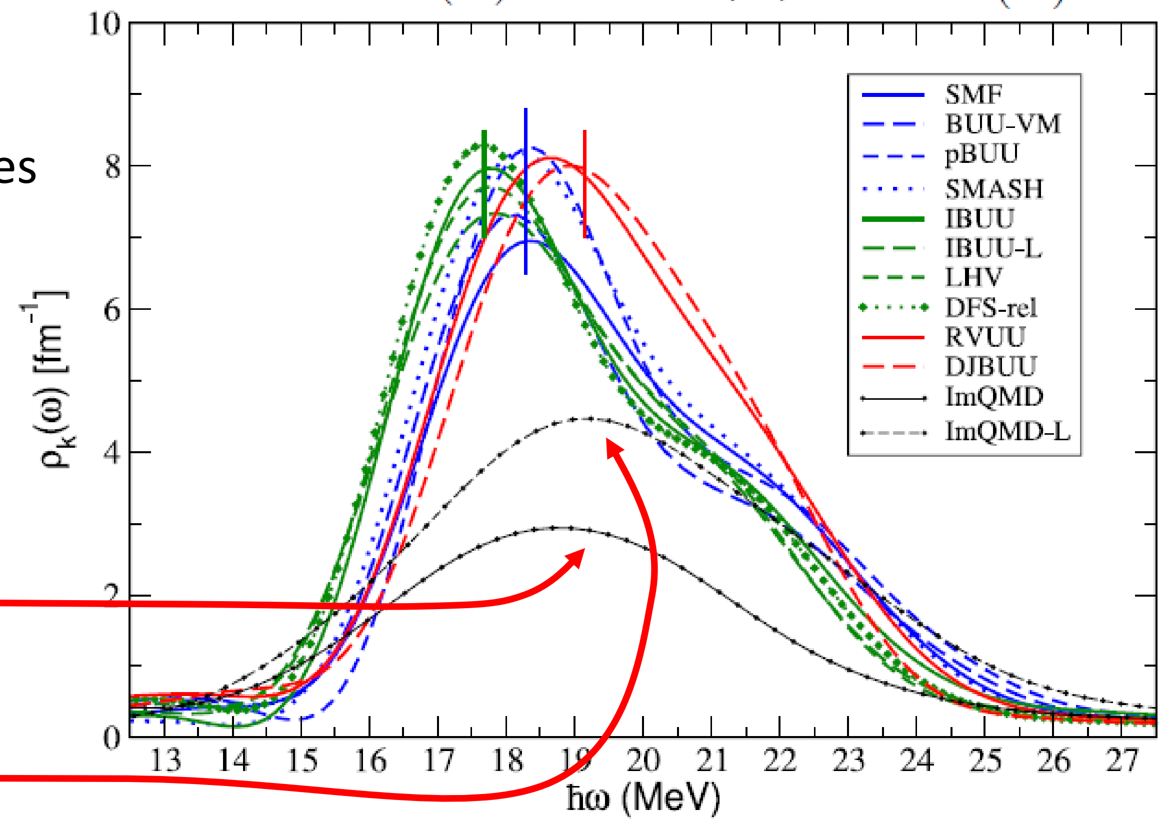
Box 1: Mean field evolution (M. Colonna, et al., PRC104 (2021))

evolution of a standing wave

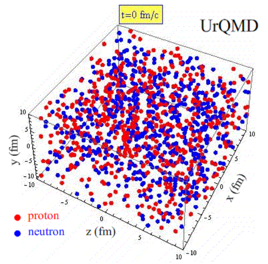


strength function, power spectrum
exact results from Landau theory: horizontal lines

Understanding diff's:
treatment of relativity (diff colors)
fluctuations affects forces, damping
treatment of non-linear term (QMD)



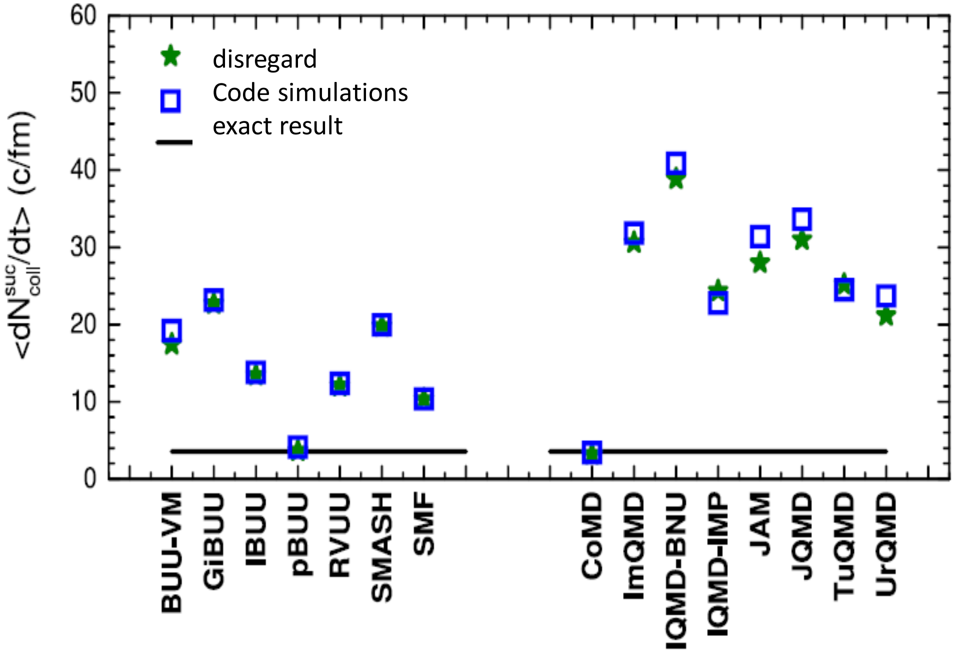
QMD traditional (Δx=1.4 fm)
more damping than BUU due to fluctuations,
shift due to approx in non-linear term
QMD-lattice, no approx.

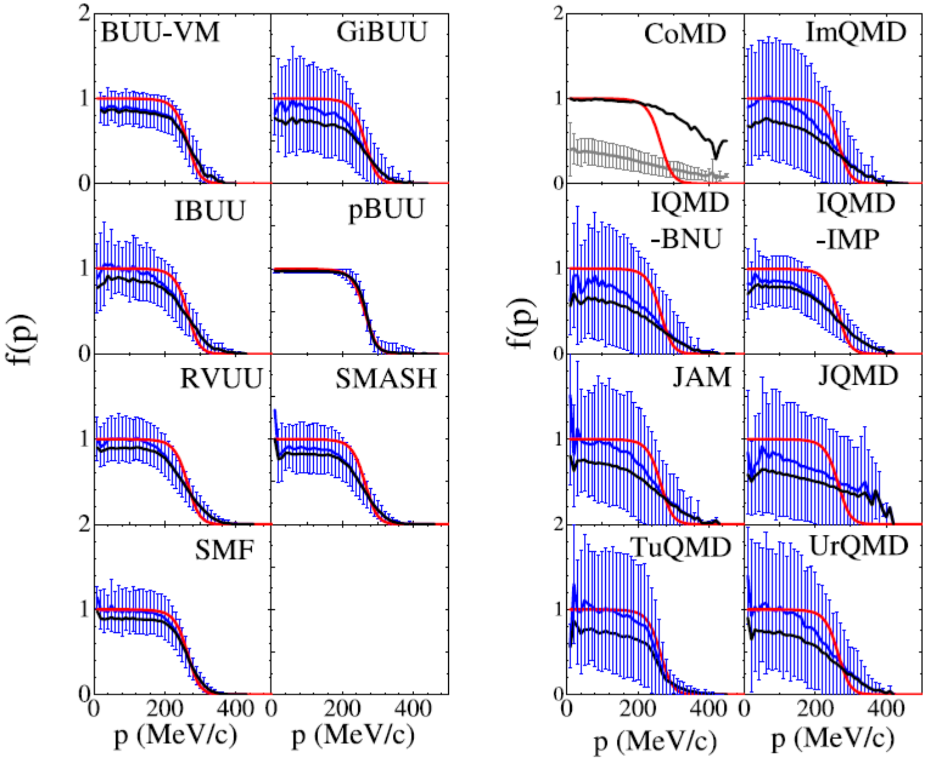


Box2: Collision intergral (only nucleons, with Pauli blocking, initialize at T=5 MeV)

(YX. Zhang, et al., PRC 97 (2018))

Collision rates, compared to exact result:
Systematic difference between BUU and QMD results





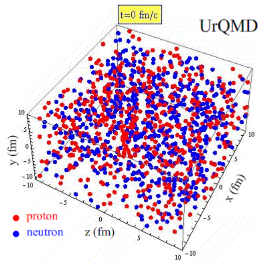
Reason: Fluctuations in Pauli blocking factor (1-f)

exact: red

average: blue

effective (enforce f≤1): black

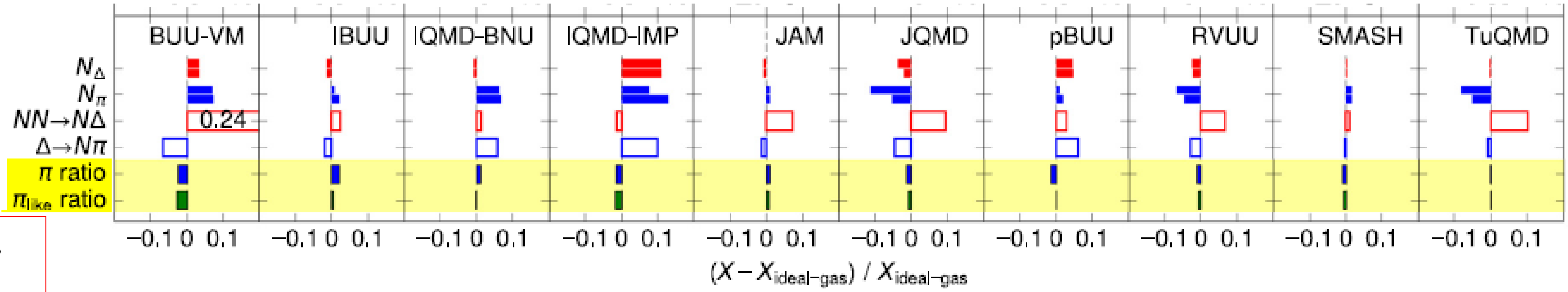
generally underblocking (black ↔ red)



Box3: Pion production in a box (w/o Pauli blocking, (A. Ono, et al., PRC 100 (2019))

extrapolation to time step zero

multiplicities and multiplicity ratios (relative difference to exact result)



determines
π−/π+ ratio
in a HIC

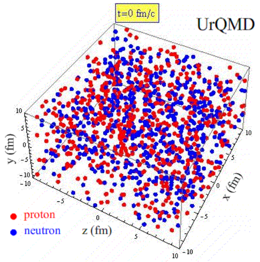
Understanding differences:

correlations between collisions (non-Markovian behavior)

geometric criterion not optimal, statistical criteria better

strategies in handling sequence of elastic and inelastic collisions

Cancel rather well in ratios

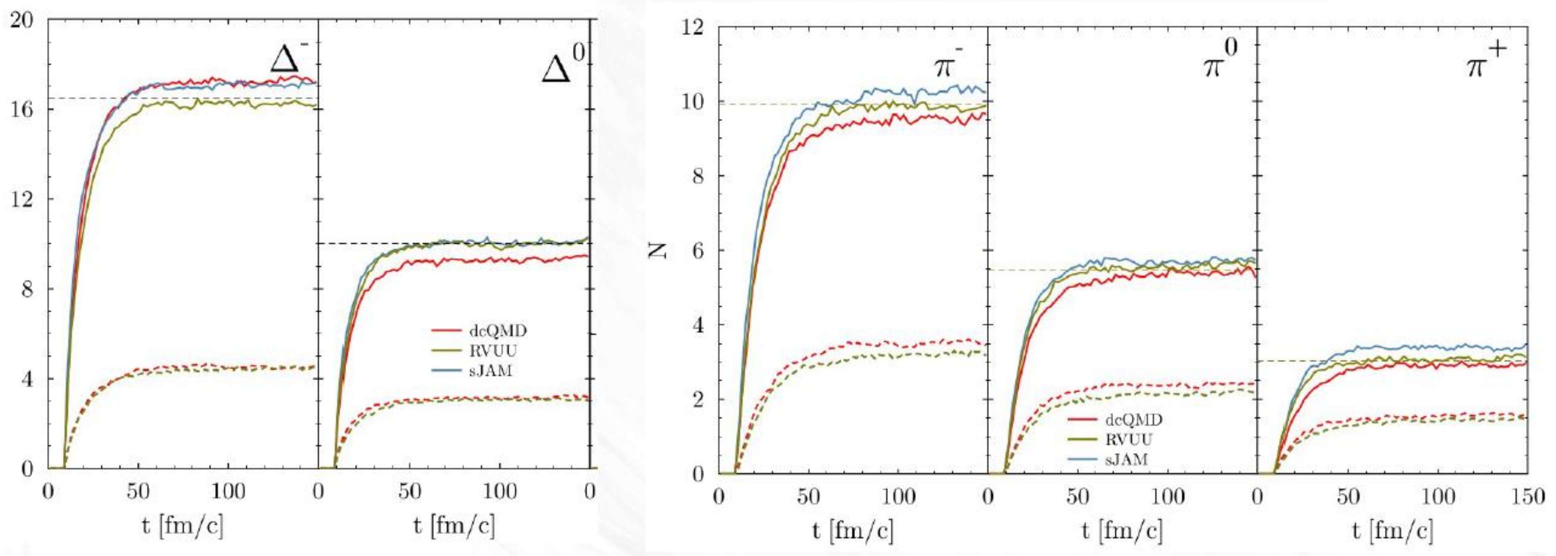


Box4: Collision integral with momentum-dependent interactions

(D. Cozma, et al., in preparation)

threshold shift in inelastic collisions with momentum dependent mean fields

4) full_mdi_th: - mean field (K_0=230 MeV; m*=0.70; $\Delta m^*_{np}/m_N$=-0.33δ; S_0=32 MeV; L=60 MeV); threshold effects included
- initialization uses effective masses (Boltzmann T=60 MeV)
- results: dcQMD, RVUU, sJAM



solid lines: with threshold effect
dashed lines: without

thin dashed line: exact result (thermal model)

rather good agreement between codes, but some deviations (being investigated)
demonstrates importance of considering threshold shift

Lessons from box calculations:

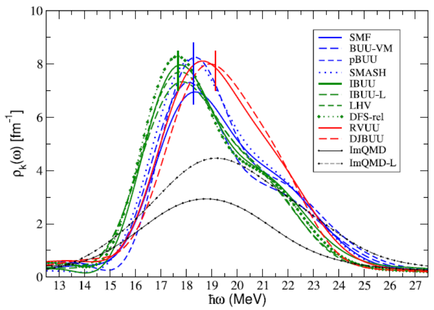
learn much about simulations,

- comparison to exact results: absolute measure of quality,
  but strategies optimized for box, may not be equally good for HIC

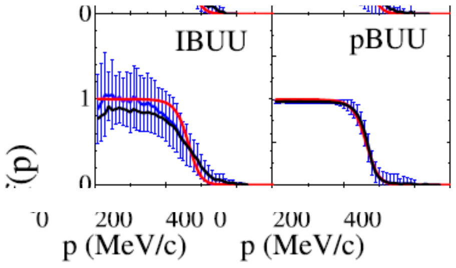
- largely understand differences between codes

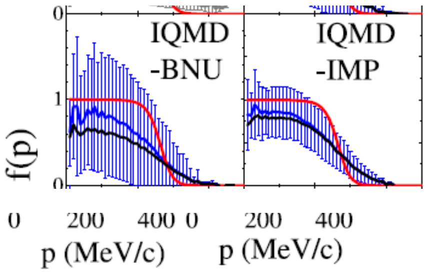
- recommend optimal strategies, e.g.
  - geometric criterion to determine next collision $d < \sqrt{\sigma(\sqrt{s})/\pi}$ may induce non-Markovian effects
    choose next collisions by statistical criteria (only implemented in some codes)

- **strong evidence of importance of fluctuations**
  - effect on calculations of mean field forces



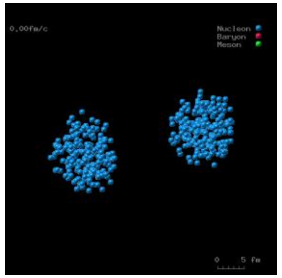
  - effect on Pauli blocking





  - affect clustering (not yet tested)

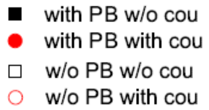
Now look at full heavy-ion collisions (HIC)



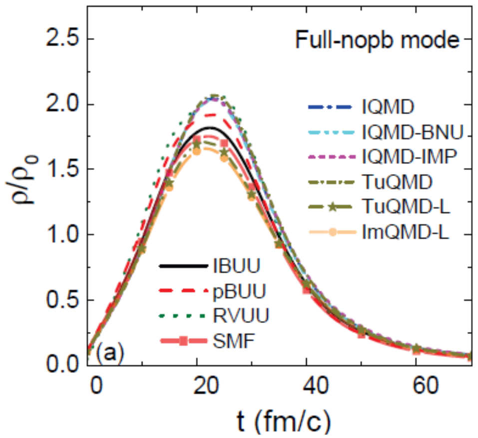
HIC: Sn+Sn@270 MeV/A (J. Xu, et al., PRC 109, 044609 (2024))

similar to Au+Au@100,400 MeV/A + pion observables

controlled input: common initializ., simple mom.-indep. EOS, σ_{el}=const, NN↔NΔ, Δ↔ Nπ

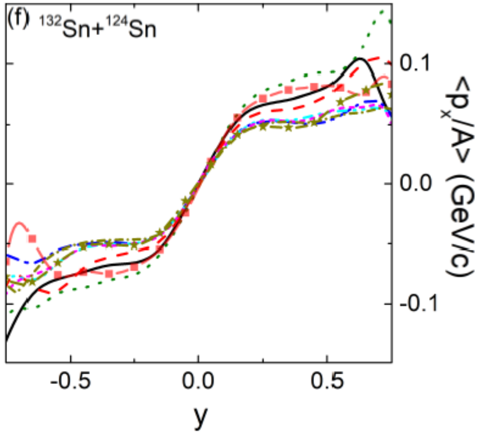


density evolution



nucleon evolution not identical, BUU codes have lower density fluctuations, approx. in non-linear term in QMD, weaker repulsion

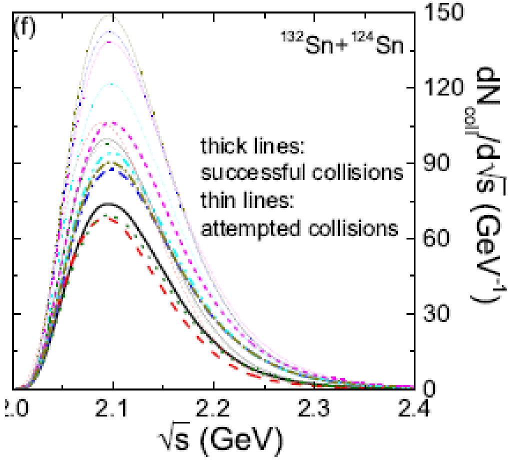
side-ward flow



correspondingly different stopping and flow

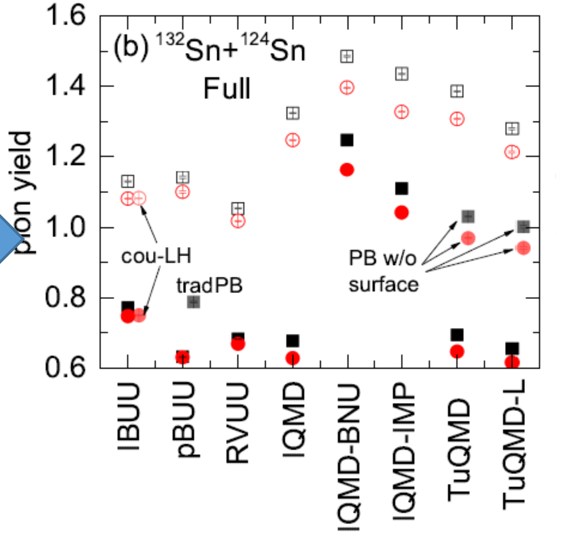
BUU codes have stronger flow

inelastic reaction rates NN→NΔ



inelastic reaction rates are correspondingly weaker in BUU

pion multiplicities



pion multiplicities

(w and w/o Pauli and Coulomb

generaly weaker for BUU

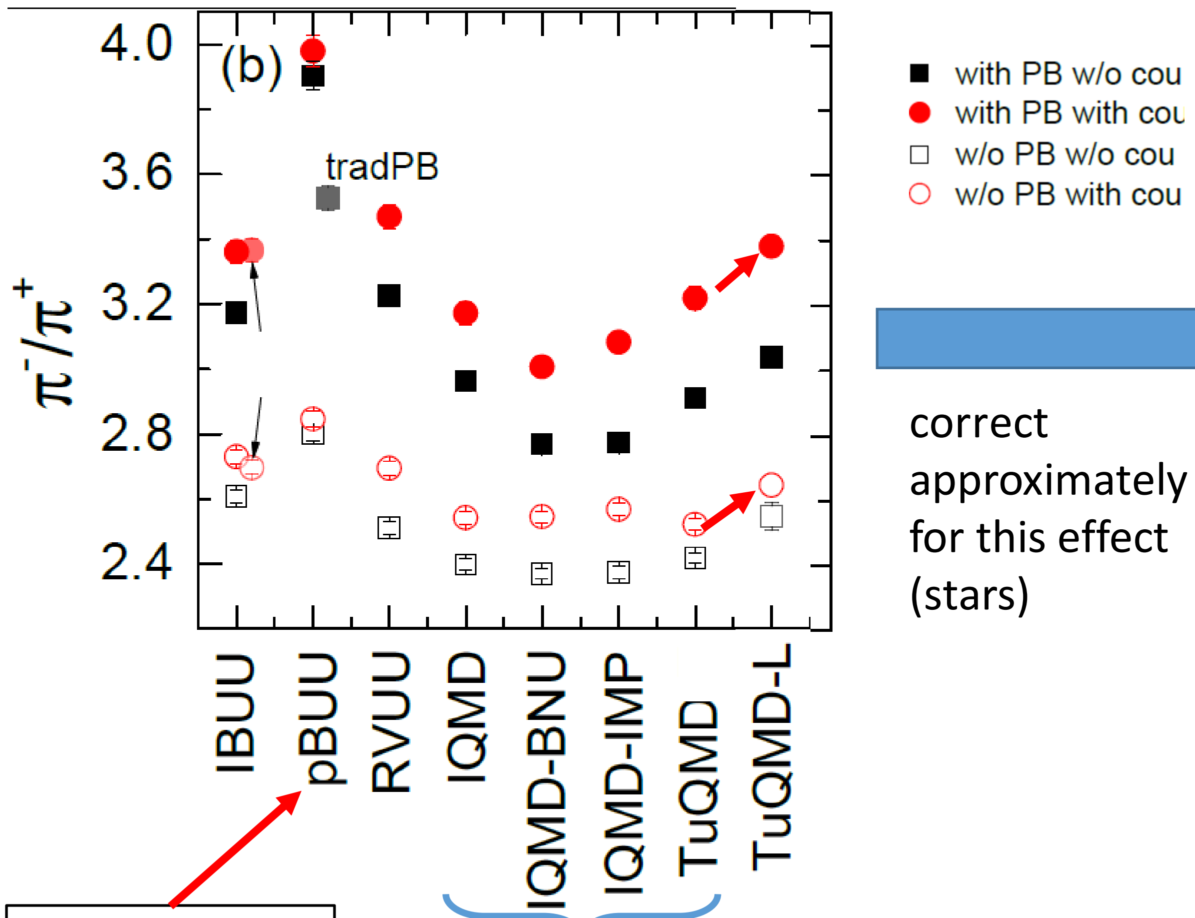
Conclusion: differences in the evolution of the system (caused here by approx. in averaging of force) leads to difference in pion observables

HIC are open systems: small differences can propagate and lead to larger final results, ingrediens interact (unlike in box)

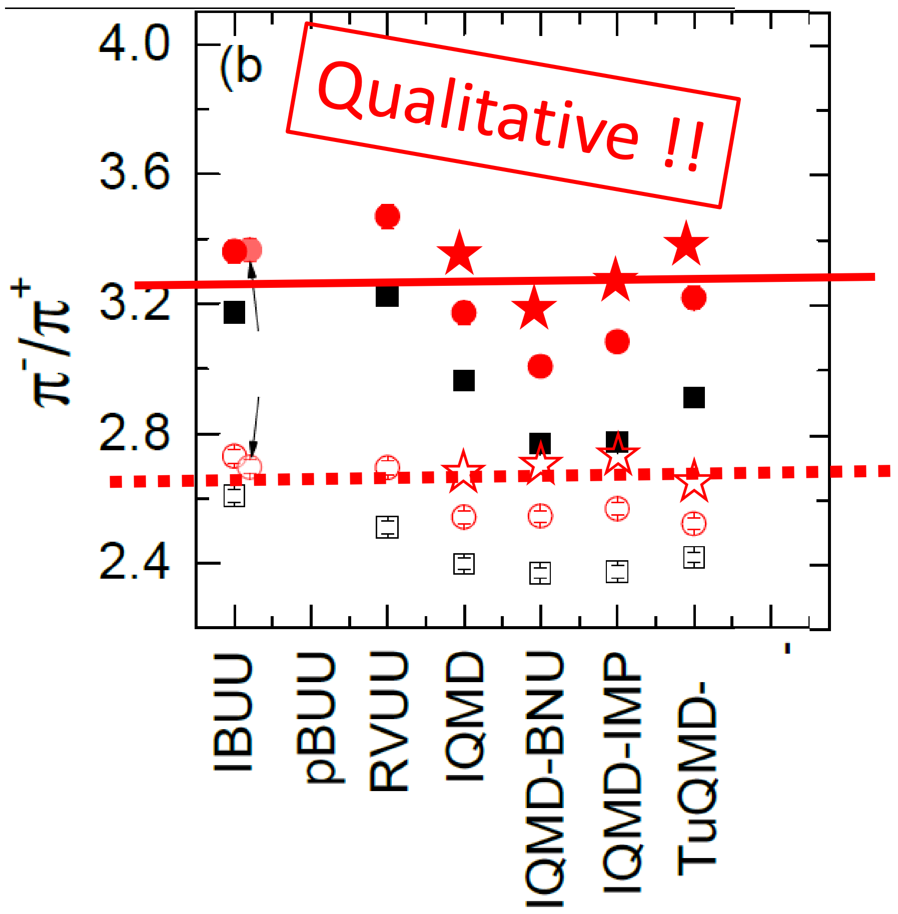
no exact results, comparison between codes, not to experiment, since (here) models are simplistic

But differences can be understood

Look closer at charged pion ratio, assumed to be a good probe for the symmetry energy



correct approximately for this effect (stars)



π, Δ feel symmetry energy not comparble

QMD codes, approx. for ρ^γ weaker repulsion, reduced pion ratio, correct by TuQMD diff.

agreement w/o Pauli-blocking very good
with Pauli-blocking differences **<≈ 10%**
(remaining differences due to Pauli blocking surgface correction)

Lessons and intermediate conclusions from Code comparisons

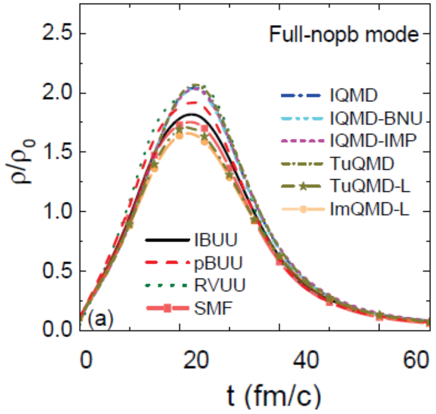
1. Code comparisons are very interesting and teach us a lot about simulation physics.
   in most cases the differences can be explained,
   but the codes often cannot be made to converge sufficiently to determine physical parameters, like J, L, K_{sym}, etc

2. Difficult to assign an error to transport results as a whole, i.e. to determine the uncertainty due to the model dependence, The mean and variance in code comparisons do not represent a reasonable error estimate.

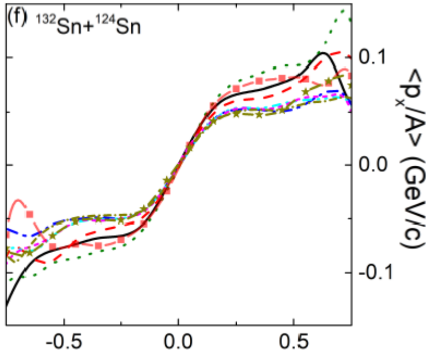
3. There are no exact results for HIC and code-to-code comparisons do not decide about the reliability of a code. But there is experiment. One can estimate the reliability of a code on it ability to describe a relevant set of experimental data (relevant to the physical question asked).

4. chain of observables

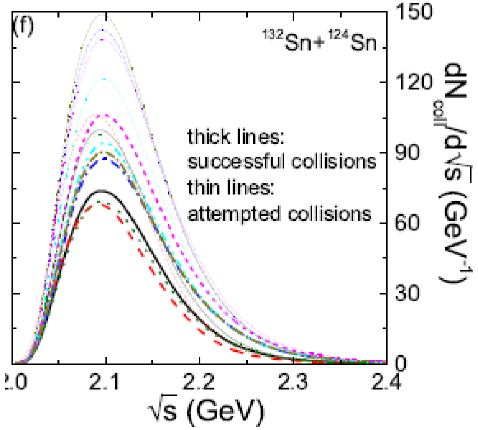
density evolution



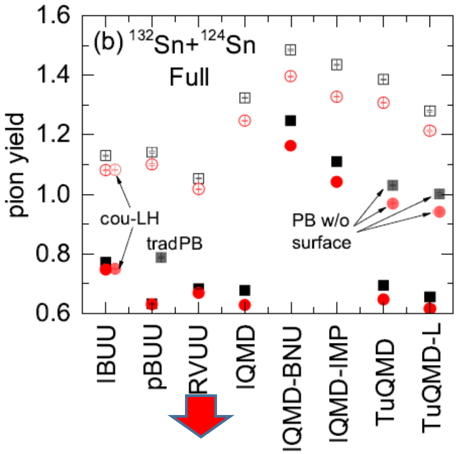
side-ward flow



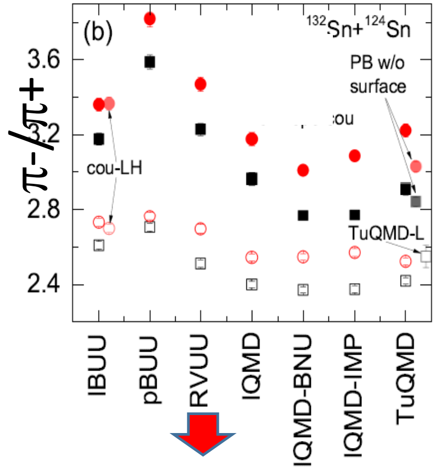
inelastic rates NN→NΔ



pion multiplicities



charged pion ratios



check with experiment

check with experiment

5. Note, that agreement with experiment is not sufficient that code is „correct“,
   but agreement with a relevant and sufficiently wide set of data does make this more probable

What is necessary for this program?

1. a realistic model, containing all necessary ingredients for the physical question, (i.e. momentum dependence of isoscalar and isovector forces, threshold shift effects, energy conservation),
2. robust computational strategies, such as converged propagation of particles, correct treatment of coarse graining, etc.

3. realistic fluctuations (strong dependence of simulation results on the amount of fluctuations),
-> make the BUU and QMD approaches compatible:
Boltzmann-Vlasov (BUU) + fluctuation term –> Boltzmann-Langevin (approximations SMF, BLOB)
Molecular dynamics (QMD) -> heuristic fluctuations and correlations, depending on a parameter (Δx)
} need to agree !

4. clustering and correlation
influences directly emission of light clusters (LC) and as seeds intermediate mass fragments (IMF)
but indirectly may influence the evoluiton of the system, and observables as pion production

many issues:
dynamical clustering (affect evolution, e.g.pBUU, Z.Zhang, R. Wang) ↔ coalescence (does not affect evolution),

- dynamical clustering:
  - explicit degree of freedom (pBUU, Z.Zhang, R. Wang)
  - Phase-space rearrangement (AMD)
  - Medium modification of clusters (Burello)
- coalescence:
  - late (freeze-out) (Gemini,..)
  - early, „dynamical“ (MST, FRIGA)

Method to implement this program: Bayesian Model Averaging (BMA).

Bayesian model inference is standard for one model, where the likelyhod is taken from this model.
What about obtaining the uncertainty for analyses with several models?
-> Bayesian model mixing with weights, which are determined from the ability of each model to describe a set data.

example: from determination of Nuclear Symmetry Energy from nuclear structure:
see talk of Mengying Qiu later

Could be applied to transport analyses of HIC to constrain the Nuclear Symmetry Energy (NSE).

1. Inferenz of NSE from Bayesian model analysis for several codes from isospin-sensitive observable.

2, Use as weights for model averaging ability to describe a relevant and sufficiently large of data on nucleon observables, e.g., stopping, flow, nucleon emission, to make sure, that reaction evolution is sufficiently well described.

3. Only then inferences from secondary observables, like pion observables, can be reasonably believed, and the averaged probabiliy distribution gives the uncertainty of transport analyses as a whole.

4. Bayesian model mixing (P. Giuliani): essentially th same, except one wants to make predictions; Uses PCA (principal component analysis) to use only essentially different models. Also useful here.

5. Possibility to also use different sets of data from structure, HIC and astrophysics

Method to implement this program: Bayesian Model Averaging (BMA).

Bayesian model inference is standard for one model, where the likelyhod is taken from this model.
What about obtaining the uncertainty for analyses with several models?
-> Bayesian model mixing with weights, which are determined from the ability of each model to describe a set data.

Could be applied to transport analyses of HIC to constrain the Nuclear Symmetry Energy (NSE).

1. Inferenz of NSE from Bayesian model analysis for several codes from isospin-sensitive observable.

2, Use as weights for model averaging ability to describe a relevant and sufficiently large of data on nucleon observables, e.g., stopping, flow, nucleon emission, to make sure, that reaction evolution is sufficiently well described.

3. Only then inferences from secondary observables, like pion observables, can be reasonably believed, and the averaged probabiliy distribution gives the uncertainty of transport analyses as a whole.

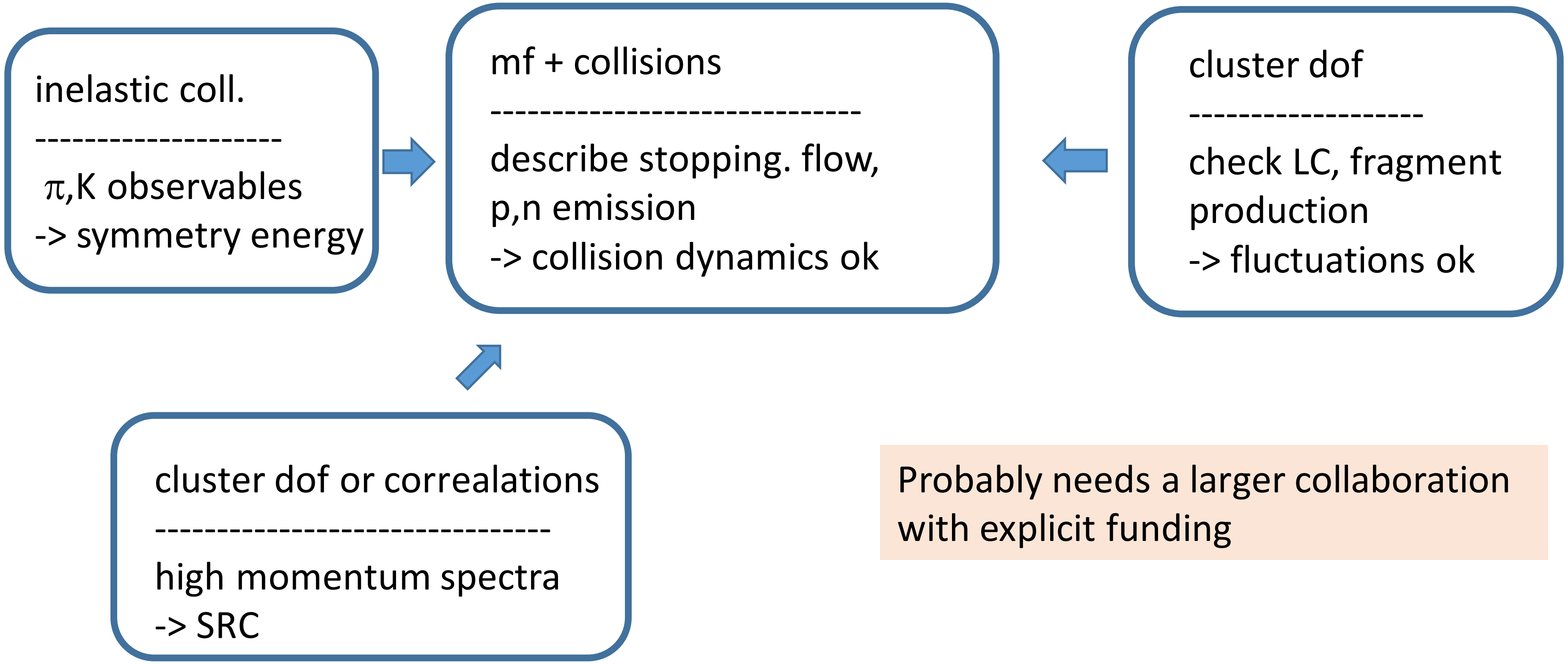
4. Bayesian model mixing (P. Giuliani): essentially th same, except one wants to make predictions; Uses PCA (principal component analysis) to use only essentially different models. Also useful here.

5. Possibility to also use different sets of data from structure, HIC and astrophysics

Alternatives:

1. Many codes, BMM

2. Construct commom code in a modular approach



Probably needs a larger collaboration with explicit funding

Summary and perspective

EOS of dense matter from HIC: extract a rather simple quantity (the bulk EOS of infinite matter) from a complicated non-equilibrium process.

However, it is the only way to obtain this information in an intermediate density regions above saturation.

bonus: obtain information not only on bulk EOS, but detailed information, like the composition, response, phase transitions, etc.

mandatory, to make use of the impressive (and costly) development of facilities and detectors

TMEP: Estimate and reduce the systematical theoretical error (the model dependence) of conclusions of transport model simulations to extract information on the EOS from heavy-ion collisions.

method: code comparisons of HIC under controlled conditions.

difficult to achieve sufficient convergence of codes to make deductions on small effects , like the nuclear symmetry energy.

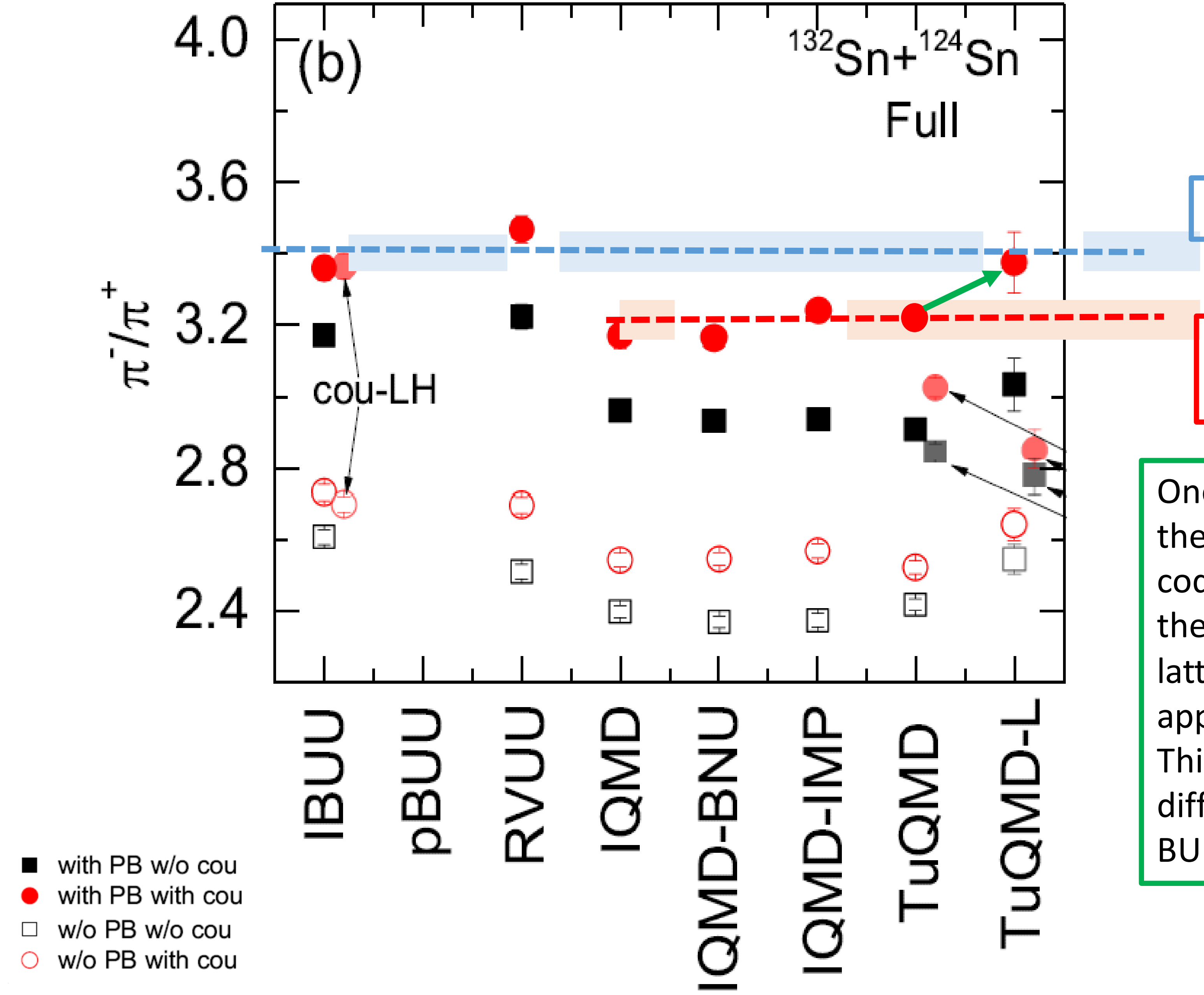
Possible ways to make progress:

- uncertainty quantification of transport analyses using Bayesian Model averaing
- code development constructing a common code in a modular approach in a dedicated collaboraion

probably funded collaboration needed

Thank you for your attention

backup



BUU-type codes, 3.40±0.05

difference 0.18

QMD-codes with surface corr 3.22±0.05 (1.8%)

One can invoke point 2b), the approximation of the non-linear term in the „traditional“ QMD codes. Its effect is seen in the difference between the TuQMD and TuQMD-L codes, because the lattice QMD method largely avoids this approximation (green arrow).
This difference (0.18) very closely agrees with the difference between the traditional QMD and the BUU-like codes (0.16).

Bayesian model averaging: Example from nuclear structure.

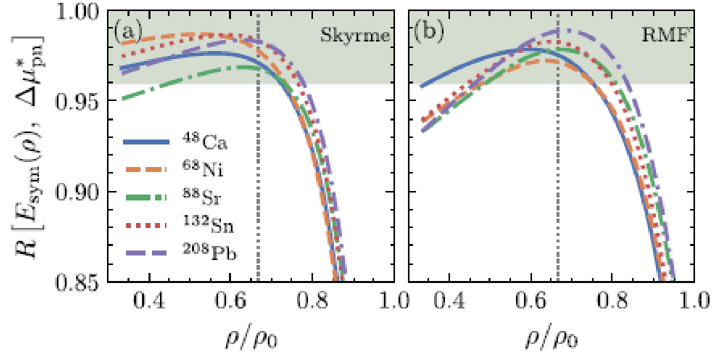
"Bayesian model averaging for nuclear symmetry energy from effective proton-neutron chemical potential difference of neutron-rich nuclei", Mengying Qiu, Bao-Jun Cai Lie-Wen Chen, Cen-Xi Yuan, Zhen Zhang, PLB 849 (24) 183435

"to extract the symmetry energy around $2\rho_0/3$ from the measured $\Delta\mu^*_{pn}$ of 5 doubly magic nuclei 48Ca, 68Ni, 88Sr, 132Sn and 208Pb"

using two models: Skyrme and RMF, each with a number of parameters.

Correlation coefficient between $E_{sym}(\rho)$ calculated for a sampling of the model space for each model and the $\Delta\mu^*_{pn}$:

-> strongest correlation with E_{sym} at $\frac{2}{3}\rho_0$



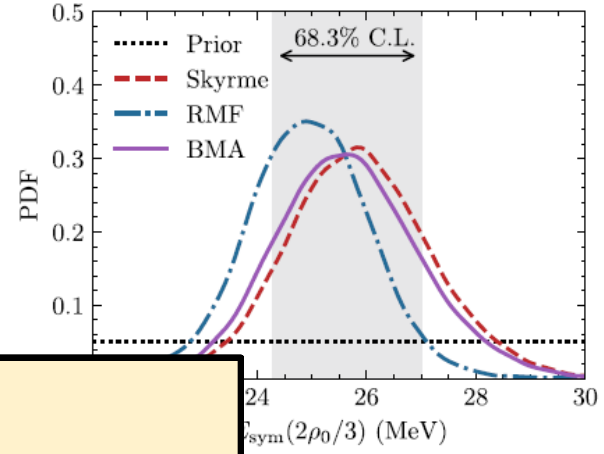
Perform Bayesian inference for each model and obtain posterior probabity distribution for Esym(2/3 ρ_0): different for the two models: mean and width.

Now average the two model with weights given by the evidence of fitting the chemical potential differences by each model Mi

$$p(\mathbf{y}\,|\,\mathcal{M}_i) = \int p(\mathbf{y}|\theta_i,\sigma_i,\mathcal{M}_i)\,\pi(\theta,\sigma|\mathcal{M}_i)\,d\theta_i\,d\sigma_i.$$

likelyhood prior

(Skyrme has a higher evidence, because the correlation is tighter, faxtor [illegible]3.)



→Obtain probability distribution of for anylsis of two models (solid line)
is Skyrme the better model? No, because evidence based on very small data set.
but if data set is enlarged, e.g. BE, radii, sp energies, the weight would be more meaningful