Evaluating Transport Models under Controlled Conditions(lessons and future directions of TMEP)





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(on behalf of TMEP collaboration)





Outline:

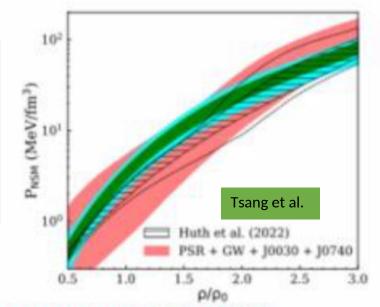
- Motivation: Increase impact of HIC studies on determination of the EOS, in particular at suprasaturation densities
- TMEP: Comparison of transport codes under controlled conditions
- box calculations: test individual ingredients, comparison to exact results, discuss lessons learned: fluctuations
- HIC: open systems, much less agreement, explanations, but difficult to quantify model dependence
- future direction of TMEP
- addional box calculations: fluctuations, mom.dep. potentials, clusterization, SRC
- Heavy-ion collisions (HICs) Uncertainty quantification:
 Bayesian inference with many codes, BMA (Bayesian model averaging)
- summary and outlook

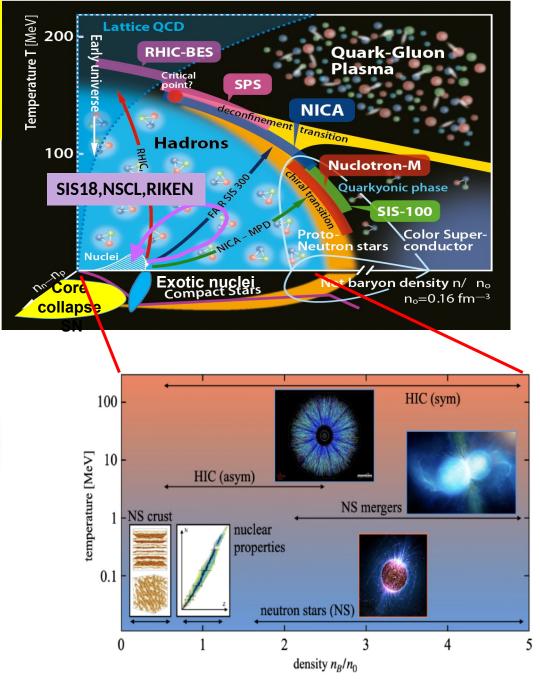
Motivation:

Importance of intermediate-energy heavy-ion collisions (HICs) for the exploration of equation-of-state (EOS) as a fct. of density **X**, temp T, asymmetry 🖗

- \rightarrow filling the gap between information from nuclear structure ($\times \leq \times_0$) and neutron star observations ($\times \otimes 2.5 \times_0$)
- -> HICs 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)

HICs are non-equilibrium processes, theoretical description complex, but based on one code. robustness of predictions is an issue.

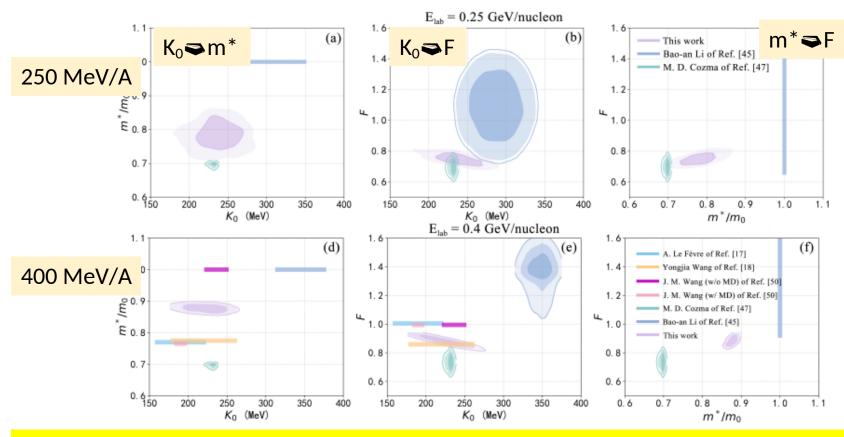




Model dependence of transport model results

non-equilibrium system-> non-equilibrium description, i.e. transport theory (Kadanoff-Baym) complex -> semiclassical approx. (Boltzmann theory; molecular dynamics)

Example: Results of different codes on values and correlations between nuclear matter parameters K₀, m*/m, F (reduction of in-medium cross section) using the same (FOPI) data (G.J. Wei, et al, arxiv 2509.03406)



same data (FOPI, Au+Au), regions of confidence do not overlap

Increase robustness of conclusions: a) comparisons of transport codes in controlled conditions (TMEP) b) not only compare but quantify uncertainty (Bayesian inference)

TMEP: compare different transport models und controlled conditions, i.e. same physical model and similar calculational parameters. but simplified physical model, no comp. to experiment

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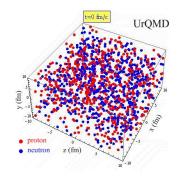


Review

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



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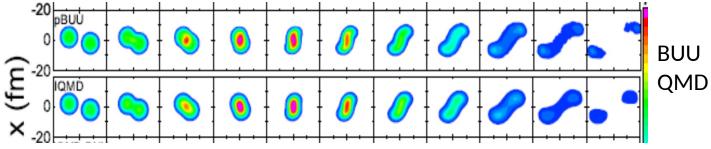


two modes of comparisons:

- box calculations, periodic boundary conditions,
 - simulates infinite nuclear matter,
 - study individually different ingredients of physical model, compare to exact limits
 - understand important aspects of transport
 - always goes to equilibrium, may not say everything for dynamic HICs



- 2. Full heavy-ion collisions (HICs), compare codes between each other,
 - substantial differences, explanations, but not sufficient convergence
 - systematic differences BUU-QMD
 - open system, small differences may cause large change in evolution



Box: Importance of Fluctuations:

$$\frac{Df(\vec{r}, \vec{p};t)}{dt} = I_{coll} \left(\sigma_{12 \to 34}^{in-med}; 1 - f_i \right) + \delta I_{fluc}$$
(Vlasov) (dissipation) (fluctuation)

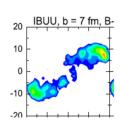
treatment of fluctuations:

1. BUU approach: Testparticles
$$f(\vec{r},\vec{p};t) = \sum_{i=1}^{n} g(\vec{r}_i - \vec{r}_i(t)) \tilde{g}(\vec{p} - \vec{p}_i(t))$$
; g TP shape, zero or finite size

 $N_{TP} \rightarrow \square$, deterministic, include flutuation term U_{fluc} , ->Boltzmann-Langevin approach N_{TP} finite, numerical fluctuations, can be gauged to physical effects, e.g. damping of collective phenomena

2. QMD approach: molecular dynamics for nucleons with finite-size wave packets: width parameter *L* regulates fluctuations event fluctuations

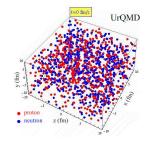
$$f(\vec{r}, \vec{p}; t) = \left(\frac{\hbar}{\sqrt{L}}\right)^{3} \sum_{i} \exp\left[-\frac{(\vec{r} - \vec{R}_{i}(t))^{2}}{2L}\right] \delta(\vec{p} - \vec{P}_{i}(t))$$



QMD event

different approximate approaches, influence results significantly not clear, what is more realistic

in the end BUU and QMD should give the similar results for EOS from same data



Box: Importance of Fluctuations: effect on blocking

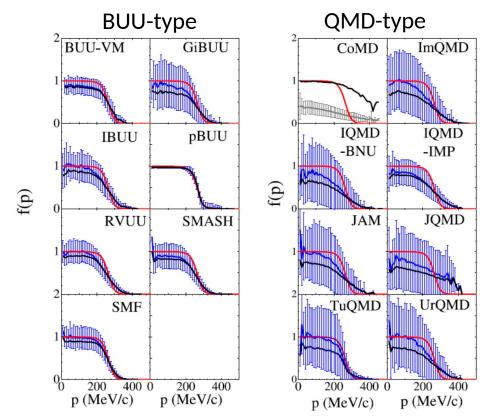
Test of collision intergral w/o mean field (only nucleons, with Pauli blocking, at T=5 MeV (YX. Zhang, et al., PRC 97 (2018))

Fluctuations in occupation of final state occupation

exact: red

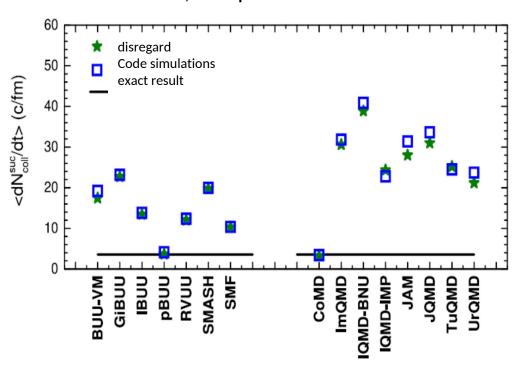
average: blue

effective (enforce f≤1): black



larger fluctuations in QMD, smaller effective occupation

Collision rates, compared to exact result:

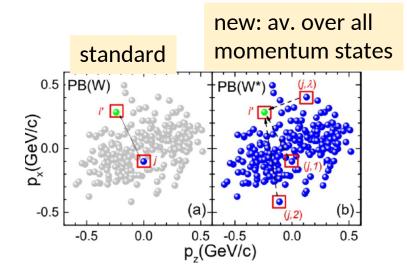


Reason: Fluctuations in Pauli blocking factor (1-f) generally underblocking (black red) systematic diffrence in BUU and QMD

Box: importance of fluctuations: example of blocking term in QMD

Study of dependence of fluctuations in QMD

X. Chen,...,YX. Zhang, A novel Pauli blocking method in quantum molecular dynamics type models, Phys.Rev.C 109, L021604 (2024) and NuSYM2025

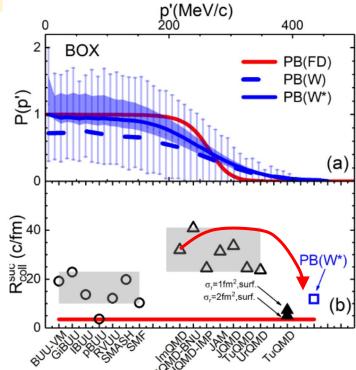


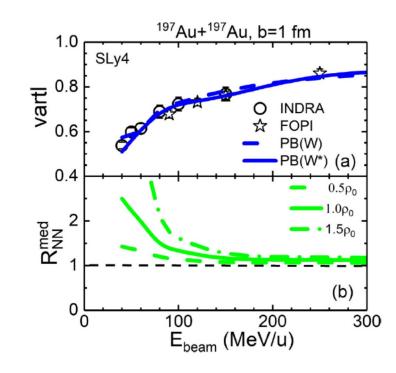
$$P_{i} = P(\mathbf{r}_{i}, \mathbf{p}_{i}')$$

$$= \frac{1}{4/h^{3}} \frac{1}{(\pi \hbar)^{3}} \sum_{j=1, j \neq i}^{N} \exp\left[-\frac{(\mathbf{r}_{i} - \mathbf{R}_{j})^{2}}{2\sigma_{r}^{2}}\right] c_{j}(\mathbf{p}_{i}'), \quad (6)$$

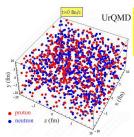
where the factor $c_j(\mathbf{p}'_i)$ is calculated as

$$c_j(\mathbf{p}_i') = \frac{1}{N} \sum_{\lambda=1}^{N} \exp\left[-\frac{(\mathbf{p}_i' - \mathbf{P}_{j,\lambda})^2}{2\sigma_p^2}\right]. \tag{7}$$





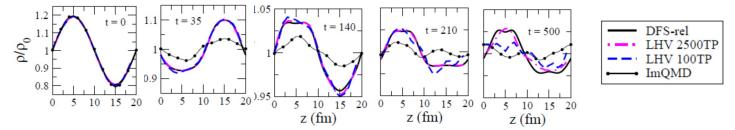
Increase of in-med Xsec to fit **vartl** with new PB -> up to factors of about 2!



Box: importance of fluctuations: influence on mean field propagation

Test of mean field evolution w/o collisions (M. Colonna, et al., PRC104 (2021))

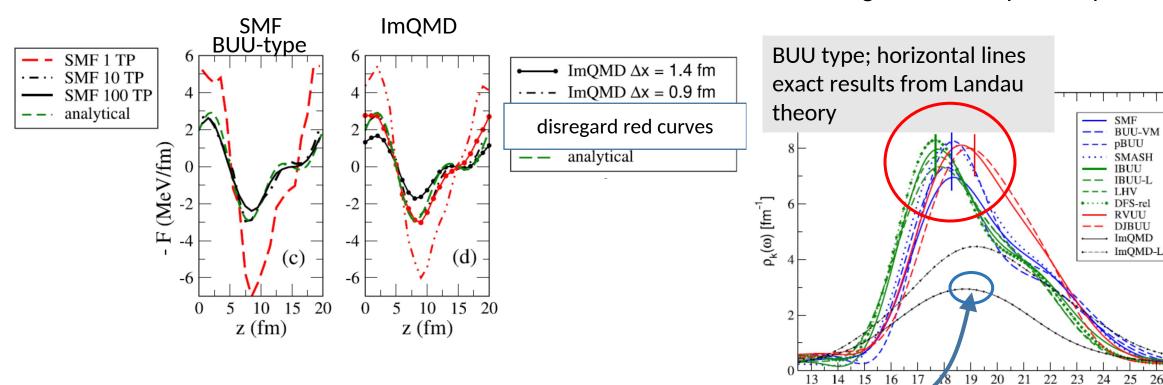
evolution of a standing wave



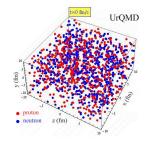
Force averaged in cells at initial time

strength function, power spectrum:

ħω (MeV)



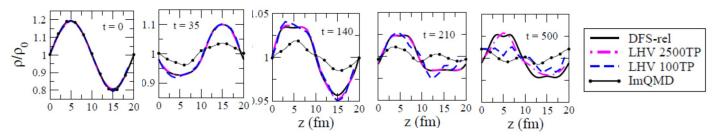
QMD codes: broadening (larger fluctuations)



Box: evaluation of mf terms: non-linear forces

Non-linear mean field evolution (M. Colonna, et al., PRC104 (2021))

evolution of a standing wave



ħω (MeV)

strength function, power spectrum: Force averaged in cells at initial time non-linear force $\langle
ho^{\gamma}
angle$ a $\langle
ho
angle^{\gamma}$ horizontal lines: exact results from **ImQMD** Landau theory $ImQMD \Delta x = 1.4 fm$ $ImQMD \Delta x = 0.9 fm$ ImQMD-L $\Delta x = 1.4$ fm SMF BUU-VM ImQMD-L $\Delta x = 0.9$ fm pBUU analytical SMASH 0 IBUU-L (black) approx. eval. of ρ^{γ} term · · · · DFS-rel **RVUU** (red) better eval. of ρ^{γ} term DJBUU lattice Hamiltonian appraoc → ImQMD --→ ImQMD-L 10 15 20 z (fm) 20 21 23

QMD codes: shift (from approximation to ρ^{γ} term) broadening (larger fluctuations)

Box: Collision Probability and Memory Effects

collision term (elastic)

$$I_{coll} = \mathbf{\hat{c}} dp_2 dp_1 dp_2 \mathbf{\hat{c}} v_{21} \mathbf{\hat{s}}_{12}^{in-med} (W) (2p)^3 \mathbf{d} (p_1 + p_2 - p_{1'} - p_{2'}) \mathbf{\hat{e}} f_{1'} f_{2'} \overline{f_1} \overline{f_2} - f_1 f_2 \overline{f_1'} \overline{f_2} \mathbf{\hat{e}} \mathbf{\hat{e}} \mathbf{\hat{c}} \mathbf{\hat{c}} \mathbf{\hat{e}} \mathbf{$$

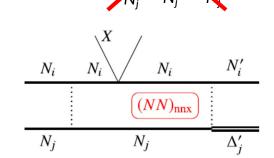
more general:
$$I_{coll} \rightarrow I_{el} (NN \leftrightarrow NN) + I_{inel} (NN \leftrightarrow N\Delta) + I_{decay} (\Delta \leftrightarrow N\pi)$$

In **kinetic theory** collision term Markovian, i.e. collisions are not correlated. In **simulations** the collision probability is treated by two methods

- 1. geometric criterion: two particles can collide if the distance is within the range given by the total cross section in a timestep. $\pi d_1^{*2} < \sigma \qquad |t_{\rm coll}^* t_0^*| < \frac{1}{2}\Delta t$
- 2. **statistical criterion:** assure that mean free path satisfies $\lambda=1/\varrho\sigma$ particles are chosen randomly in a cell and their collision proapility is

method 1 has to be supplemented to avoid **repeated collisions** by the same particles in subsequent steps. However, **higher order correlations** may occur, e.g. in an inelastic collisions with an intermediate interaction with a third particle.

other effects may be due to the **order** in which elastic, inelastic and decay processes are treated. This was found to influence and and multiplicities

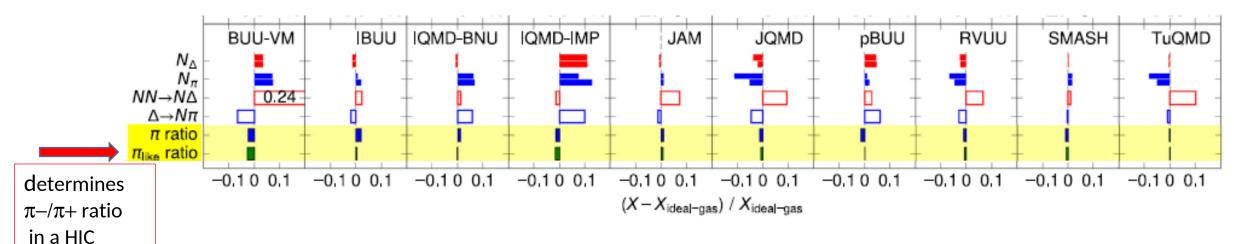


 $P_{ij}(\Delta t) \approx \varrho \sigma v_{ij} \Delta t$

Box 2: collision probability and memory effects

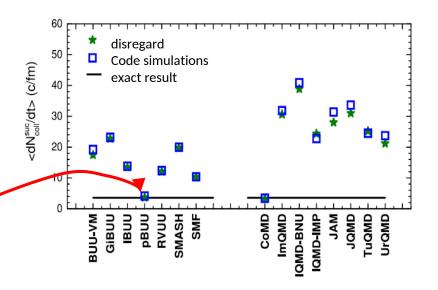
proton on cutron z (fm)

test of pion production in a box w/o Pauli blocking, cascade (A. Ono, et al., PRC 100 (2019)) extrapolation to time step zero multiplicities and multiplicity ratios (relative difference to exact result)



Understanding differences:

- correlations between collisions (non-Markovian behavior)
- geometric criterion induces correlations
- strategies in handling sequence of elastic and inelastic collisions
- Cancel rather well in ratios in a box
- statistical prescription (e.g. pBUU) works very well in box



Box calculations: lessons

fluctuations affect evolution of HIC substantially:

less effective blocking, force calculation in mf propagation

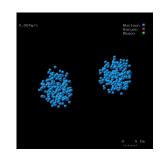
memory effects

Simulations using geometrical criteria for the collision probility induce correlations, cannot be completely eliminated, and are very dependent on strategies in the collision term Have an effect on multiplicities of secondary particles but perhaps strict Markovian behavior is an idealization?

other effects (not yet studied in box calculation):

fluctuations are seeds for cluster correlations and light cluster production (also for fragment formation)

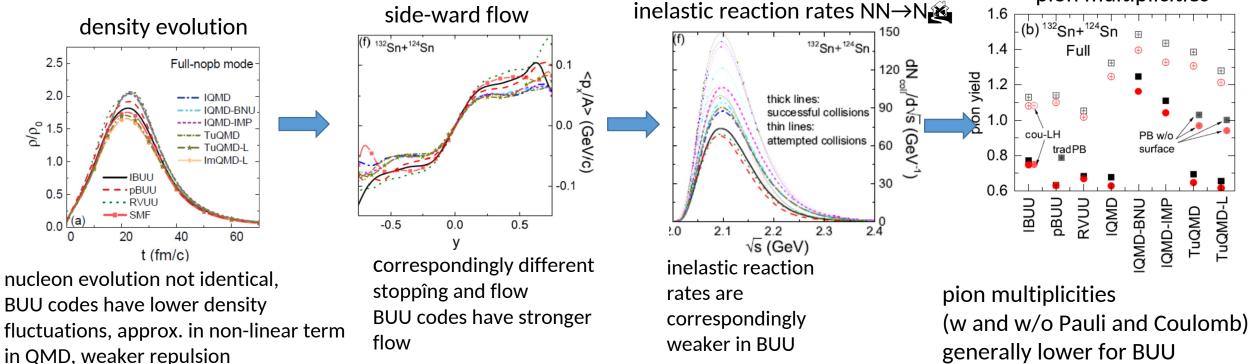
-> important insights into transport smulations from box calculations concern major open problem in treatment of HICs



Comparison of HICs: open system

 with PB w/o couwith PB with couw/o PB w/o couw/o PB with cou

pion multiplicities



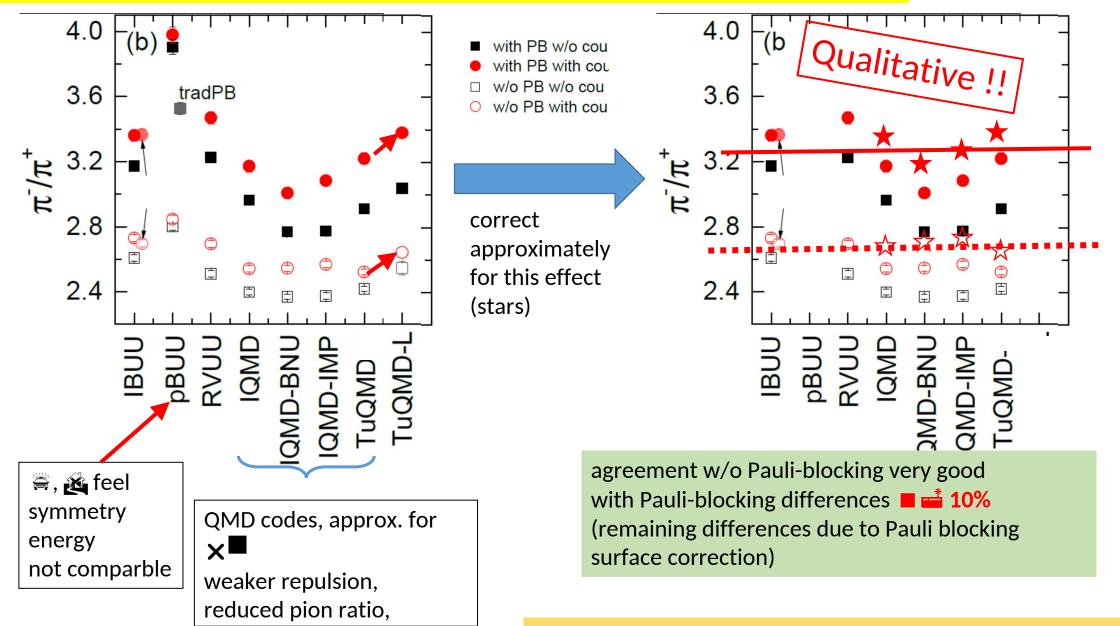
Conclusion: differences in the evolution of the system, leads to difference in pion observables

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

But differences can be understood

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

correct by TuQMD diff.



Thus, can explain differences, but how to quantify uncertainties

Intermediate conclusion for code comparisons:

box calculation:

- we learn a lot about simulations of transport codes
- in particular we discussed the importance of fluctuations and of memory effects
- we can compare to exact limits, and in most cases satisfy these or understand deviations
- box calculations test equilibrium conditions, but not dynamic properties

HICs:

- we find considerable differences, which we can mostly explain. residual differences are < 10%
- but we cannot eliminate them, and it is not clear, what is best.
- open systems, surface effects
- uncertainty estimates between code are difficult
- one probably should go beyond mere comparisons of codes

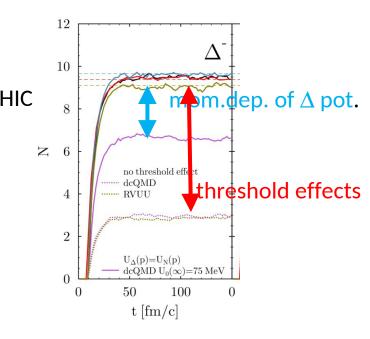
ideas of future projects for TMEP:

- further box calculations to test some more critical ingredients of transport
- HIC: uncertainty quantification

Further **box comparisons**:

- momentum dependence of the potentials, pre-requisite for a realistic description of HIC on-going study (Dan Cozma) including pion degrees-of-freedom compare to thermal model (equilibrium) results: mom.-dependence changes results substantially, threshold effects non-resonant pion production important at low pion energies
 - 2. fluctuations in a box.

exact limits from Laundau theory in the small amplitude limit insights on the different approaches of BUU and QMD on fluctuations



variance $\sigma_k^q = T/F^q(k)$, where $F^q(k) = (\frac{\partial U_k^q}{\partial \rho^q} + 1/\mathcal{N})$

 U_k = Fourier transform of the mean-field potential $\mathcal{N} = -\frac{4}{(2\pi)^3} \int d\boldsymbol{p} \, \frac{\partial f_0}{\partial \epsilon}$

$$\mathcal{N} = -\frac{4}{(2\pi)^3} \int d\mathbf{p} \, \frac{\partial f_0}{\partial \epsilon}$$

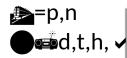
3. clusterization

compare perturbative (coalescence) and dynamic (light cluster as explicit degrees of freedom) approaches

medium effects on clusters (Mott effect)

$$\langle f_{\tau} \rangle_{\nu}(\vec{P}) \equiv \int \tilde{f}_{\tau} \left(\frac{\vec{P}}{A} + \vec{q} \right) |\phi_{\nu}(\vec{q})|^{2} d\vec{q} \leqslant F_{A}^{\text{cut}}$$

A larger F_A^{cut} corresponds to a weaker Mott effect



Momentum distribution of the constituent nucleons, related to the light-nuclei internal wave function

Heavy-ion collisions: Uncertainty quantification of transport results

- go beyond mere comparisons
- try to quantify uncertainty of results not only from a single code, but from several codes,
- no exact results, use experiment as a reference
- → comparative Bayesian inference

sketch possible steps and requirements

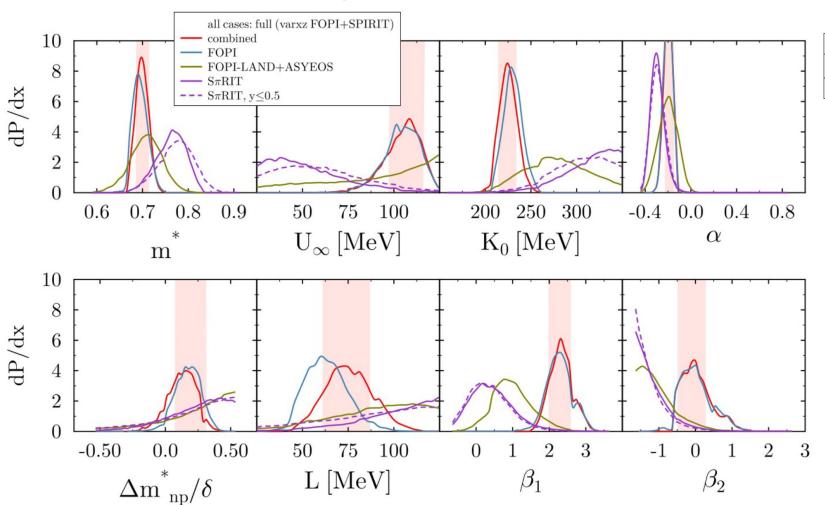
Bayesian inference with realistic models: steps

- 1. Collect codes, that have all the physical ingredients for a realistic description of intermediate energy HIC,
- mom.-dependence, symmetry energy, effective masses and n/p mass differences, medium modifications of Xsecs
- physical models not necessarily identical parametrization, but should allow to vary the physical properties
- BUU and QMD codes (if possible also BL and AMD),
- not necessarily very many, but willing to make modifications
- 2. codes should satisfy benchmark calculations in box simulations
- 3. Select observables sensitive to the EOS and dynamical properties
- sufficiently complete data should exist, which include stopping and flow as functions of (y,p_T) for a sufficiently large range of energies to allow to asses a range of densities and several systems (asymmetry effects)
- one could start with a subset of data and with a smaller set of parameters and expand subsequently,
- 4. Each code makes a **Bayesian inference** on the given set of data. obtains **probability density distributions (PDFs)** for the chosen EOS properties. sensitivity of the chosen EOS properties to data given by width of marginalized PDFs could be published individually for each code

Bayesian Inference: posterior Probability Distributions Functions (PDFs)

Example: Extensive Bayesian inference by Dan Cozma with the code dcQMD using FOPI, FOPI-LAND, ASY-EOS, and SpiRIT data on flow (v_1 , v_2 , varxz, y and p_T -spectra, and stopping: D . Cozma, arXiv 2407.16411, PRC 110 (2024)

PDFs for EOS parameters using different data sets



	FOPI	combined
K ₀ [MeV]	230 ± 10	225 ± 10
L [MeV]	63 ±10	74 ± 13

The PDFs are strongy influenced by the choice of the data.

The width of the PDF give the intra-model uncertainty of the parameters by the given data.

Narrow PDFs signify a strongly constraining observable for the respective parameter, thus the **sensitivity** of an observable.

This is important information, but is derived from only one code, i.e. is model dependent.

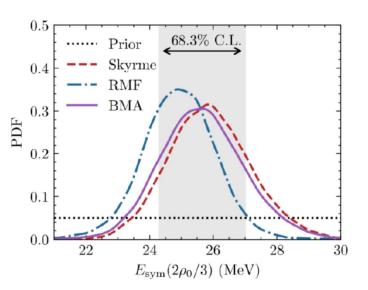
Comparative Baysian inference (Bayesian Model Averaging, BMA):

- PDFs of different codes are compared
- they are combined in a Bayesian model averaging (BMA) with weights,
- which depend on the goodness of the optimal fit
- the averaged PDFs give the result of transport anlyses on the EOS as a whole and its uncertainty

Bayesian model averaging

- lacktriangle Model prior $\pi(M_i)$: our preference on M_i before seeing the data.
- ♦ Model likelihood: (pseudo-)evidence $Z_i = p(y | M_i)$
- ♦ Model averaging for observable \mathcal{O} : $p(\mathcal{O} | \mathbf{y}) = \sum_{i} p(\mathcal{O} | \mathbf{y}, M_i) p(M_i | \mathbf{y})$

Example from nuclear structure (M. Qiu,..,Z.Zhang, PLB849, 183435 (24)) BMA for the inference from data of proton-neutron chemical potential differences $\Delta\mu_{pn}^*$ on the symmetry energy at density $E_{sym}(2/3~\rho_0)$ for two models Skyrme and RMF



width of BMA gives uncertainty of $E_{\text{sym}}(2/3\rho_0)$ taking into account two structure models

Comparative Baysian analysis: Observables

- primary observables, that determine the bulk properties of matter: nucleonic (n,p,LC) complete: flow, stopping (y, p_T; asymetry ♥, density X)
- understand and control first

secondary observables: pionic (\equiv , \bowtie), strange (K, ?) depend strongly on bulk description, reasonably complete similar as nucleonic data, avoid ratios or double ratios, reduce sensitivity issues:

- 🚔 ,🚵 potentials, momentum dependent
- resonant, non-resonant \(\beta\) production mechanism (Cozma)
- anti-strange mesons are good messenger of the dense phase

Summary and outlook

TMEP project to evaluate codes by comparison of results with unified input

- 1. box calculations, comparison to exact equilibrium results
 - learn much about critical aspects of transport simulations
 - particular important: role of fluctuations
 - future box studies: fluctuations, momentum dependence, clusterization, short-range correlations
- 2. **HICs**, comparison between codes
 - differences in open systems
 - possible to explain difference, residual difference estimated <10%
 - not possible to quantify model dependence
- 3. one possible way to go: Comparative Bayesian inference
 - realistic models, "complete" as possible set of data, Bayesian inference for each code
 - Baysian model averaging with weight, depending on quality of universal fit
 - **uncertainty due to model dependence**

other possible way: develop common modular code in a community effort (EMMI?)

Establish HICs as an indispensible way to constrain the EOS

Thank you for your attention