

Nusym2016, Beijing,  
June 13-17, 2016



# Understanding transport simulations of heavy-ion collisions at intermediate energies

-Comparison of heavy-ion transport codes under controlled condition

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J. Xu, L.W. Chen, B. Tsang, H. Wolter,  
Y.X. Zhang *et al.* (31 authors),  
Phys. Rev. C 93, 044609 (2016)  
arXiv : 1603.08149 [nucl-th]

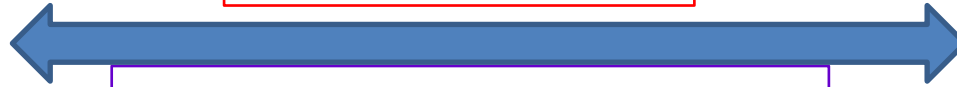
18 transport codes: 9 BUU + 9 QMD

**Nuclear EOS,  $E_{\text{sym}}$**



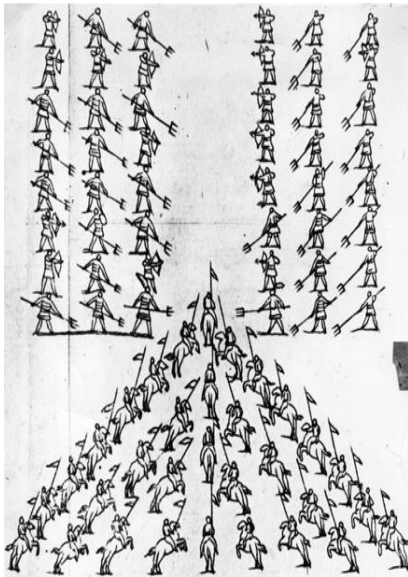
**Mean-field potential**

**How reliable?**



**Heavy-ion experiments**

**Transport simulations**



**Initialization**



**Mean Field**



**NN scatterings**

**theoretical uncertainties?**

**Compare results from various models**

# History of Transport Model Comparison Project

- **Trento I (2003):** energy 1-2 GeV/A, emphasis on particle production  $\pi, K$

mean field and Pauli blocking not quite so important

Summary Published in **J.Phys. G31 (2005) 741**

- **Trento II (2009):** energy 100, 400 MeV/A

Uncertainties not well understood

results not published

# Transport2014 in Shanghai



International Workshop on Simulations of Low and Intermediate Energy Heavy Ion Collisions (Transport 2014)

January 8-12, 2014, Shanghai, China

**Mainly 100 AMeV, also 400 AMeV**

**observables: stopping, flow**

**Nonobservables: stability, scattering and Pauli blocking rate**

# Participating Codes

## Boltzmann-Uehling-Uhlenbeck(BUU)-type models (9)

BUU-type	code correspondents	energy range	reference
BLOB	P.Napolitani,M.Colonna	0.01 ~ 0.5	[19]
GIBUU-RMF	J.Weil	0.05 ~ 40	[20]
GIBUU-Skyrme	J.Weil	0.05 ~ 40	[20]
IBL	W.J.Xie,F.S.Zhang	0.05 ~ 2	[21]
IBUU	J.Xu,L.W.Chen,B.A.Li	0.05 ~ 2	[11, 22]
pBUU	P.Danielewicz	0.01 ~ 12	[23]
RBUU	K. Kim,Y.Kim,T.Gaitanos	0.05 ~ 2	[24]
RVUU	T.Song,G.Q.Li,C.M.Ko	0.05 ~ 2	[25]
SMF	M.Colonna,P.Napolitani	0.01 ~ 0.5	[26]

In GeV

Find representative references for each code in arXiv: 1603:08149 [nucl-th]

# Participating Codes

## Quantum-Molecular-Dynamics(QMD)-type models(9)

QMD-type	code correspondents	energy range	reference
AMD	A.Ono	0.01 ~ 0.3	[27]
IQMD-BNU	J.Su,F.S.Zhang	0.05 ~ 2	[28]
IQMD	C.Hartnack,J.Aichelin	0.05 ~ 2	[29, 30]
CoMD	M.Papa	0.01 ~ 0.3	[31]
ImQMD-CIAE	Y.X.Zhang,Z.X.Li	0.02 ~ 0.4	[32]
IQMD-IMP	Z.Q.Feng	0.01 ~ 10	[33]
IQMD-SINAP	G.Q.Zhang	0.05 ~ 2	[34]
TuQMD	D.Cozma	0.1 ~ 2	[35]
UrQMD	Y.J.Wang,Q.F.Li	0.05 ~ 200	[36, 37]

In GeV

ImQMD-GXNU: low-energy fusion reaction

Find representative references for each code in arXiv: 1603:08149 [nucl-th]

# A taste of BUU-type models

**BUU equation:** 
$$\left( \frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla_{\vec{r}} - \nabla_{\vec{r}} U \cdot \nabla_{\vec{p}} \right) f(\vec{r}, \vec{p}; t) = I_{coll}[f; \sigma_{12}]$$

$$I_{coll} = \frac{1}{(2\pi)^6} \int dp_2 dp_3 d\Omega |v - v_2| \frac{d\sigma_{12}^{med}}{d\Omega} (2\pi)^3 \delta(p + p_2 - p_3 - p_4) \\ \times [f_3 f_4 (1 - f)(1 - f_2) - f f_2 (1 - f_3)(1 - f_4)]$$

## test-particle (TP) method: parallel events

C.Y. Wong, PRC 25, 1460 (1982); G.F. Bertsch and S. Das Gupta, Phys. Rep. 160, 189 (1988).

## Point particle or finite size (triangular, Gaussian)

$$f(\vec{r}, \vec{p}; t) = \frac{1}{N_{TP}} \sum_{i=1}^{N_{TPA}} g(\vec{r} - \vec{r}_i(t)) \tilde{g}(\vec{p} - \vec{p}_i(t))$$

**Equation of motion from pseudoparticle method:**

$$d\vec{r}_i/dt = \nabla_{\vec{p}_i} H; \quad d\vec{p}_i/dt = -\nabla_{\vec{r}_i} H.$$

# A taste of QMD-type models

Total wave function as products of single-particle wave function:

$$\Psi(\vec{r}_1, \dots, \vec{r}_N; t) = \prod \phi_i(\vec{r}_i; t),$$
$$\phi_i(\vec{r}_i; t) = \frac{1}{(2\pi)^{3/4}(\Delta x)^{3/2}} \exp \left[ -\frac{(\vec{r}_i - \vec{R}_i(t))^2}{(2\Delta x)^2} + i\vec{r}_i \cdot \vec{P}_i(t) \right]$$

Wigner function (phase-space distribution):

$$f_i(\vec{r}, \vec{p}) = \frac{1}{(\pi\hbar)^3} \exp \left[ -\frac{(\vec{r} - \vec{R}_i(t))^2}{2(\Delta x)^2} \right] \exp \left[ -\frac{(\vec{p} - \vec{P}_i(t))^2 \cdot 2(\Delta x)^2}{\hbar^2} \right]$$

Canonical equation of motion:

$$d\vec{R}_i/dt = \nabla_{\vec{p}_i} H, \quad d\vec{P}_i/dt = -\nabla_{\vec{r}_i} H$$

Ch. Hartnack et al., PRC 495, 303 (1989); J. Aichelin, Phys. Rep. 202, 233 (1988).

**AMD and FMD: wave function antisymmetrized**



# Homework description:

## Initialization and reaction parameters

### 2) Reaction:

Initial coordinate space: Woods-Saxon distribution

a) Au + Au, at 100 A MeV

b) Initialization: Initialize your (test)particles to obtain in coordinate space a Fermi function density profile with radius  $R=xA^{1/3}$  ( $x=1.12$  fm) and diffuseness  $a=0.6$  fm. In case you are using finite size (test)particles, use a sphere of the above radius and try to adjust the width in such a way as to approach the diffuseness (if possible).

The momentum of the particles should then be chosen randomly in the local Fermi sphere.

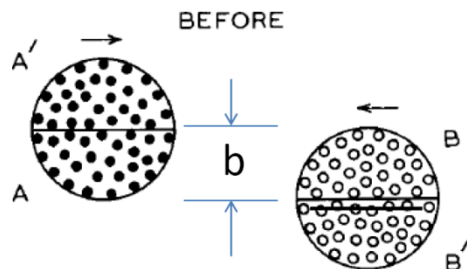
c) impact parameter  $b=7$  and  $20$  fm, with initial distance (between the centers of project and target) in z-direction  $16$  fm

d) number of runs and (test)particles:

BUU: 10 runs, 100 TP/nucleon (for finite size TP), 500 TP/nucleon (for point TP)

MD: 1000 runs.

e) time evolution: run until  $t=140$  fm/c. Use the time step you are usually using. For a second order integration method we suggest  $0.5$  fm/c.



**$b=7$  fm: real collisions**

**$b=20$  fm: single nucleus evolution-stability**

# Homework description:

## Mean-field potential and NN scattering

### 1) Physical input parameters:

#### a) Equation-of-state:

For non-relativistic transport codes: use a standard *soft Skyrme* parametrization (without momentum dependence) with the following parameters:

$a = -209.2$  MeV,  $b = 156.4$  MeV,  $\tau=1.35$ ,  $M=938$  MeV

with a symmetry potential energy with linear density dependence  $S_{\text{pot}}^*(\rho/\rho_0)$ ,  $S_{\text{pot}} = 18$  MeV.

The total single-particle potential is then:

$$U_{n/p} = a(\rho/\rho_0) + b(\rho/\rho_0)^\tau \pm 2S_{\text{pot}}^* \rho/\rho_0 \delta \quad (\delta = (\rho_n - \rho_p)/\rho)$$

(Properties of this parameterization: Compression modulus  $K_0=240$  MeV, saturation density  $\rho_0=0.16$  fm<sup>-3</sup>, binding energy at saturation density  $E_0 = -16$  MeV, symmetry energy  $S(\rho_0) \sim 30.3$  MeV)

For relativistic transport codes: use a *nonlinear  $\sigma$ - $\omega$ - $\rho$  RMF* parameterization “*NL $\rho$* ”

(see parameter set I in PRC65, 045201, by Liu B et al.)

(properties of this parameterization:  $K_0=240$  MeV,  $\rho_0=0.16$  fm<sup>-3</sup>,  $E_0=-16$  MeV,

$S(\rho_0) \sim 30.3$  MeV)

b) use a constant isotropic elastic cross section of 40 mb.

c) turn off all inelastic collisions.

# Homework list for code contributors

Mode A). Homework1

Mode B). Au+Au@100 AMeV

**B.1) No Surface Term mode:** Turn off the surface term in the mean field (e.g., the Yukawa interaction in the QMD-like models, the gradient term in the BUU-like models). Allow collisions between all nucleons (or TP).

**B-Full: both mean field and NN scattering**

**B.2) Vlasov mode:** Turn off all collisions and use mean field as in B.1 (no surface terms)..

**B-Vlasov: only mean field**

**B.3) Cascade mode:** Turn off all interaction potentials in B.1 mode

**B-Cascade: only NN scattering**

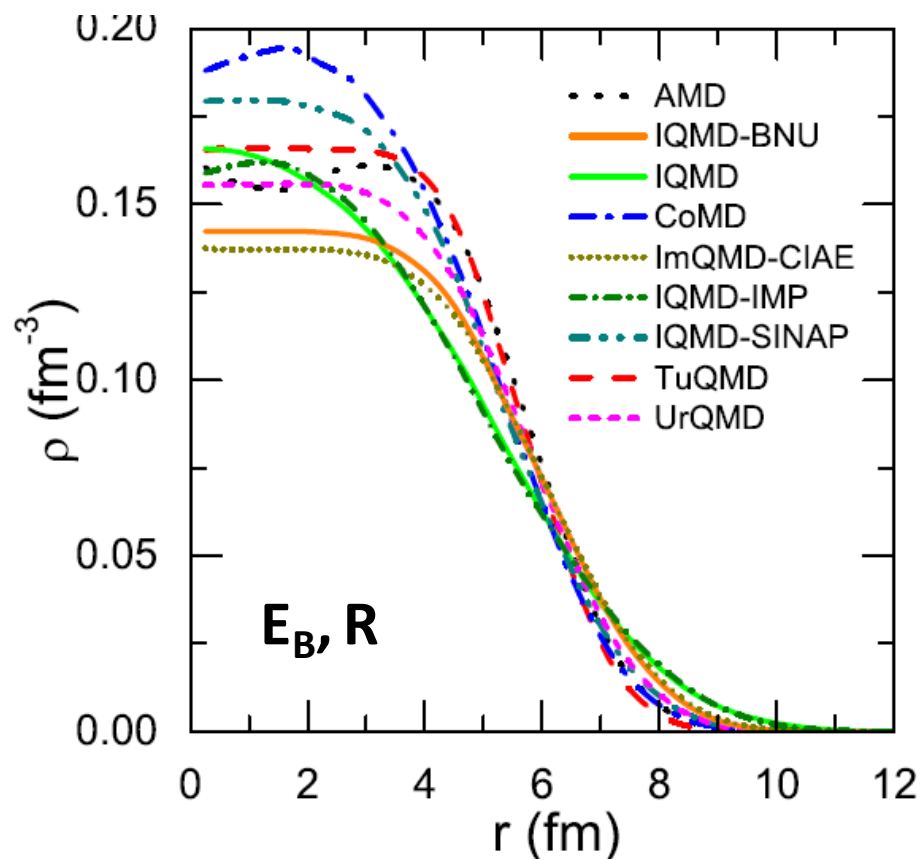
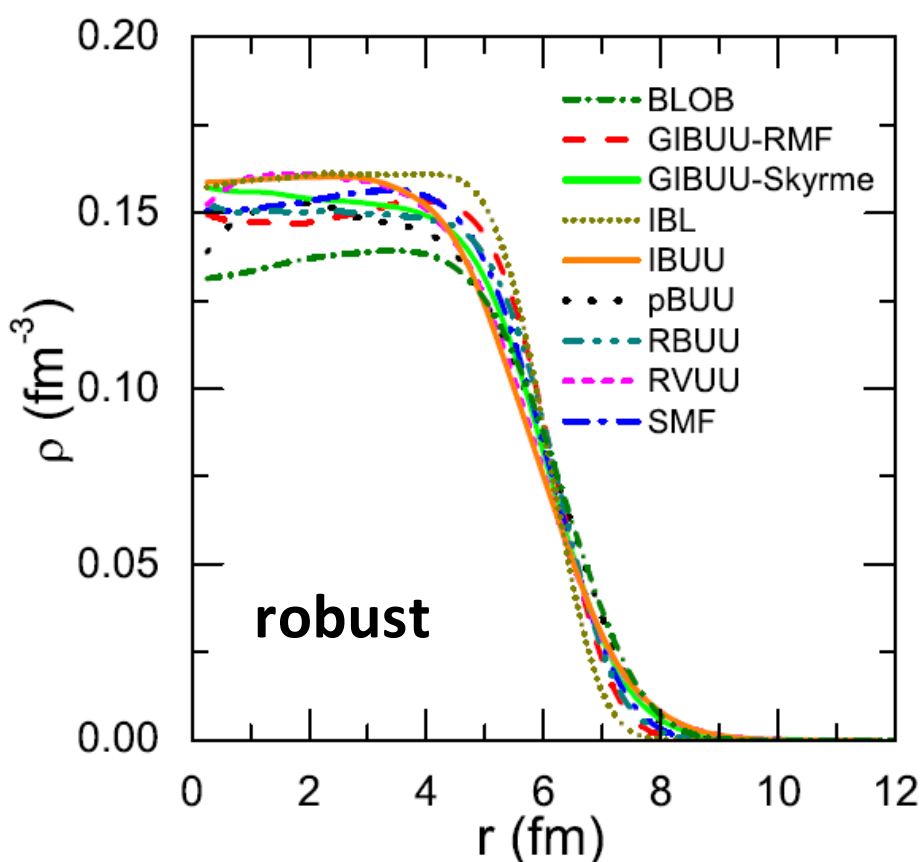
Mode C). Common initialization

Mode D). Au+Au@400 AMeV

**D-Full: 400AMeV, both mean field and NN scattering**

Mode E). Box calculation

# Initial density profile








**average over 1000 events**

**BUU: mostly follow the suggested Woods-Saxon distribution, easily stable**

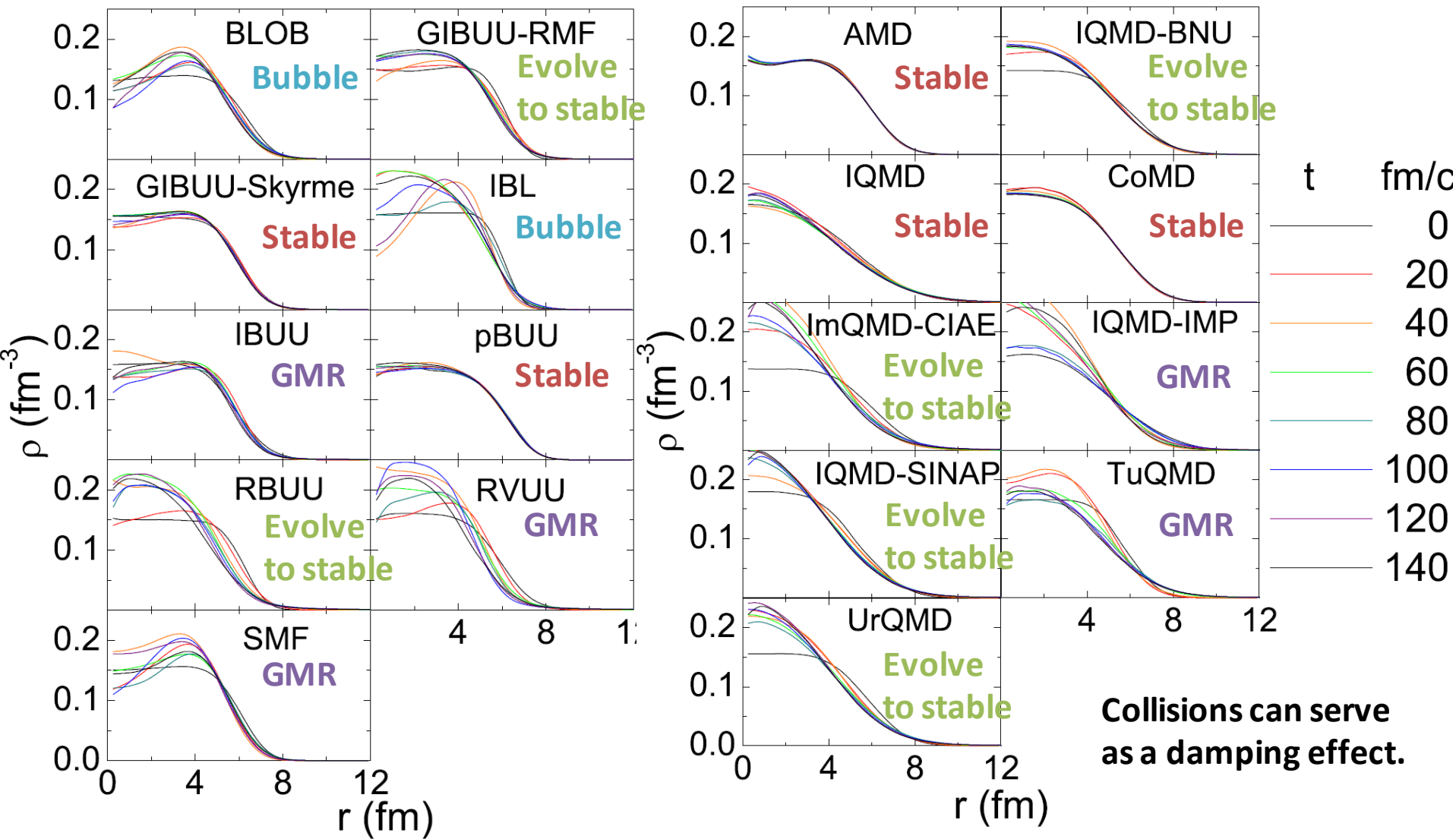
**QMD: mostly deviate from the suggested Woods-Saxon distribution**

**ground state? Thomas-Fermi or Hartree-Fock, frictional cooling**

**Difficult to get a common initialization**

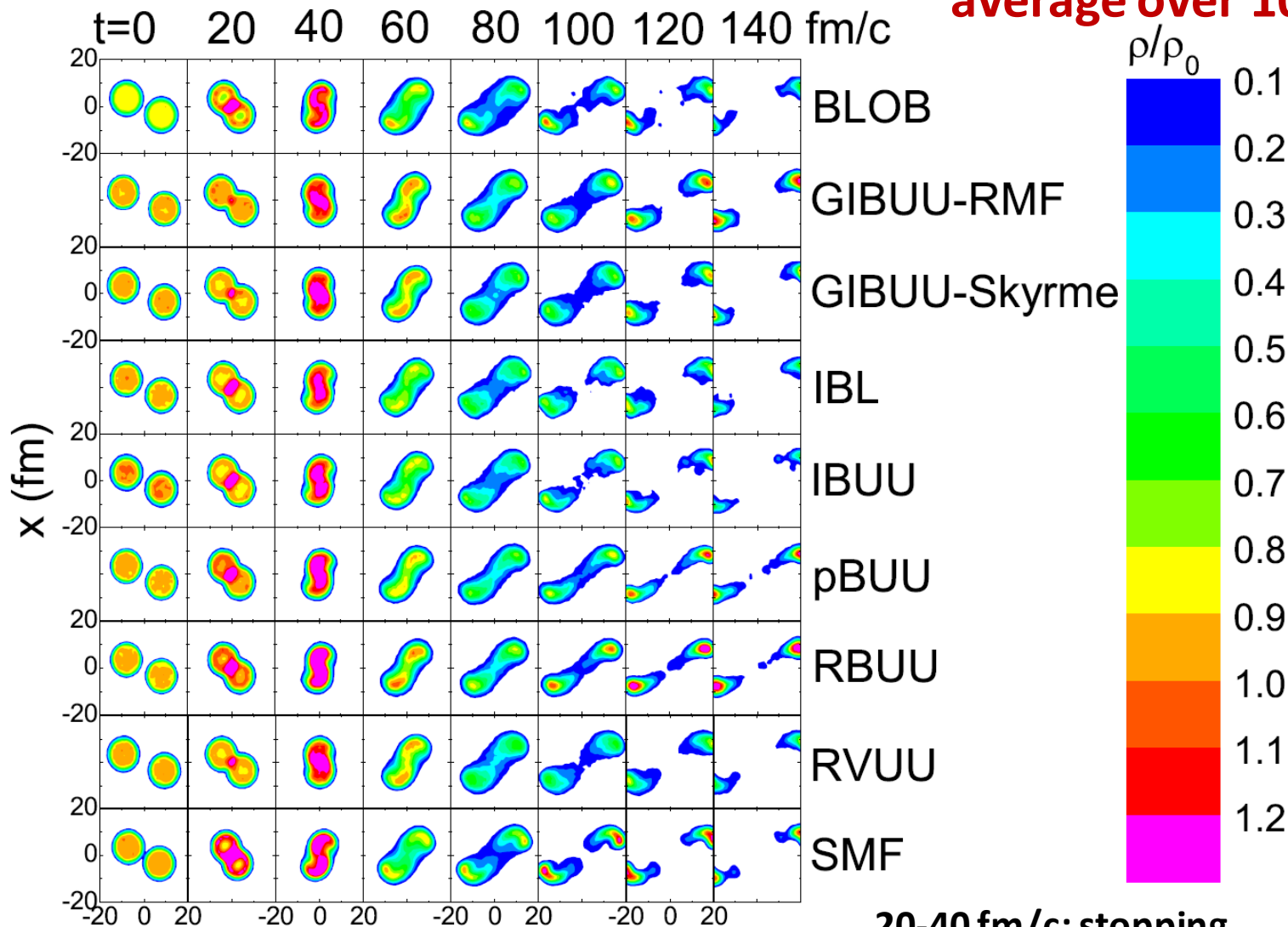
Code name	Shape of particles	$(\Delta x)^2(\text{fm}^2)^a$ Size of particles		$\delta\langle r^2 \rangle^{1/2}(\text{fm})^b$ $\langle r^2 \rangle^{1/2} - \langle r^2 \rangle_{\text{WS}}^{1/2}$	$\delta\langle r^4 \rangle^{1/4}(\text{fm})^c$ $\langle r^4 \rangle^{1/4} - \langle r^4 \rangle_{\text{WS}}^{1/4}$
AMD	Gaussian	1.56		-0.01	0.01
IQMD-BNU	Gaussian	1.97		0.32	0.39
IQMD	Gaussian	2.16		0.64	0.85
CoMD	Gaussian	1.32		-0.11	-0.04
ImQMD-CIAE	Gaussian	2.02		0.39	0.47
IQMD-IMP	Gaussian	1.92		0.61	0.80
IQMD-SINAP	Gaussian	2.16		0.03	0.12
TuQMD	Gaussian	2.16		-0.17	-0.17
UrQMD	Gaussian	2		0.12	0.18
	Shape of test particle	$(\Delta x)^2(\text{fm}^2)$ or $l(\text{fm})^f$ Size of test particles			
BLOB	Triangle	2		0.10	0.07
GIBUU-RMF	Gaussian	1		-0.18	-0.26
GIBUU-Skyrme	Gaussian	1		-0.03	-0.03
IBL	Gaussian	2		-0.32	-0.42
IBUU	Triangle	1		0.01	0.04
pBUU	Point	0 <sup>g</sup>		0.01	-0.02
RBUU	Invar. Gauss	1.4		-0.12	-0.19
RVUU	Point	0		0.01	0.03
SMF	Triangle	2		-0.13	-0.18

# Stability (b=20 fm)



# Density evolution at $b = 7$ fm - BUU

average over 1000 events



high  $\rho \Rightarrow$  high  $\rho$

Density  $\Rightarrow$  attempted collisions, mean field

Pauli blocking  $\Rightarrow$  successful collisions

20-40 fm/c: stopping

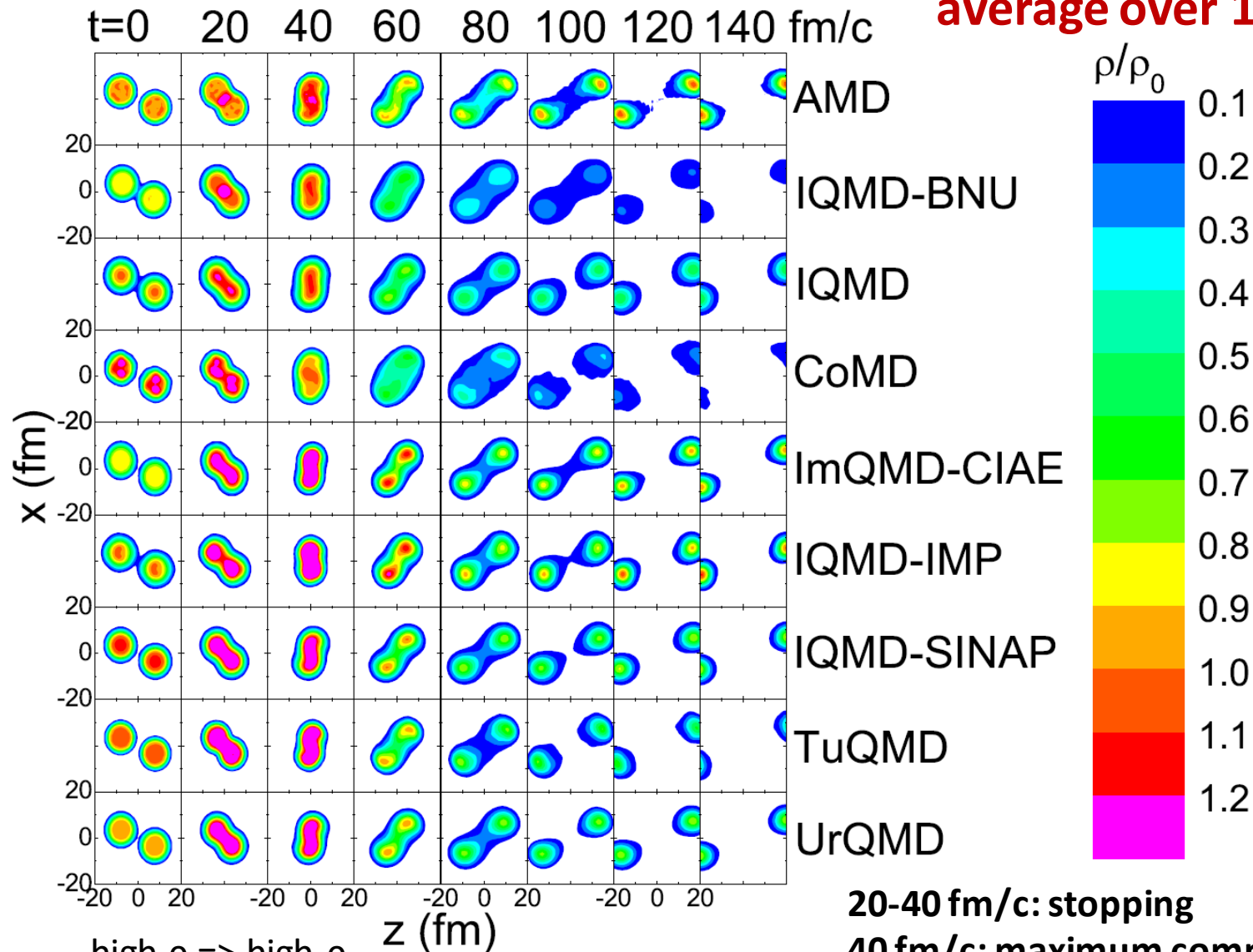
40 fm/c: maximum compression

60-80 fm/c: sideward flow developed

Around 100 fm/c: neck

# Density evolution at $b = 7$ fm - QMD

average over 1000 events



high  $\rho \Rightarrow$  high  $\rho$

Density  $\Rightarrow$  attempted collisions, mean field

Pauli blocking  $\Rightarrow$  successful collisions

20-40 fm/c: stopping

40 fm/c: maximum compression

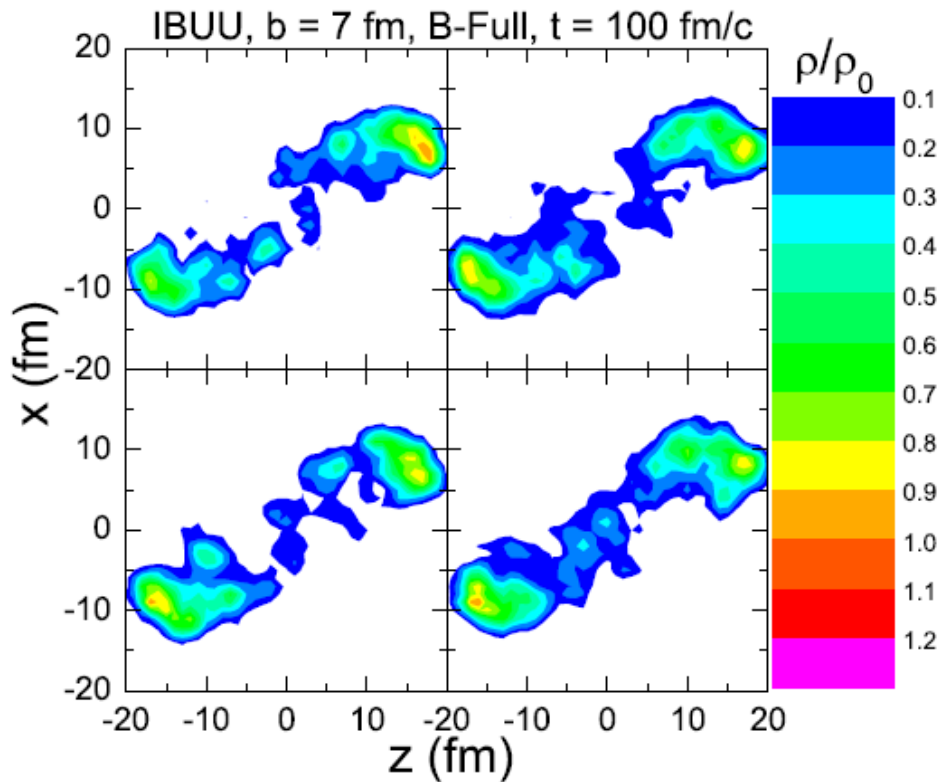
60-80 fm/c: sideward flow developed

Around 100 fm/c: neck



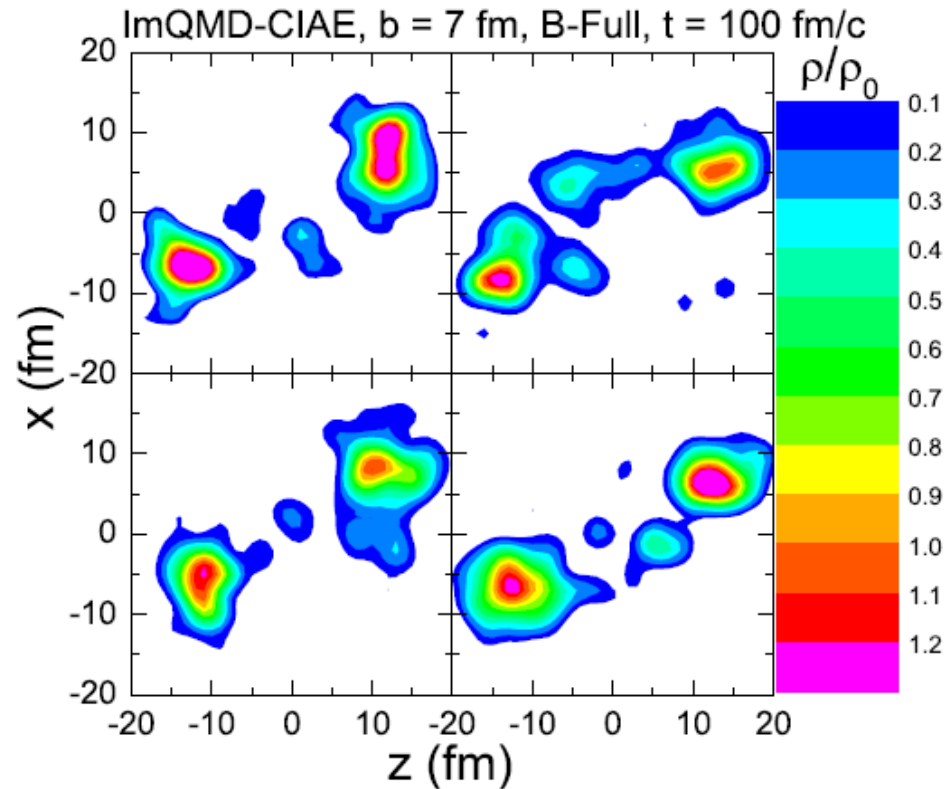
# Fluctuation in BUU and QMD

4 runs with 100 TPs per nucleon



Fluctuation related to  $N_{TP}$

4 individual events



Fluctuation related to the Gaussian width

# How are the collisions realized?

## (in most transport models)

- Bertsch's approach (Phys. Rep. 160, 189 (1988))

- Go into the C.M. frame of the two nucleons

- Collision can happen if

$$b = \sqrt{(\Delta \mathbf{r})^2 - (\Delta \mathbf{r} \cdot \mathbf{p}/p)^2} < \sqrt{\sigma/\pi} \quad \text{and} \quad \left| \frac{\Delta \mathbf{r} \cdot \mathbf{p}}{p} \right| < \left( \frac{p}{\sqrt{p^2 + m_1^2}} + \frac{p}{\sqrt{p^2 + m_2^2}} \right) \delta t/2$$

- If collision happen, change the direction of  $\mathbf{P}_{\text{cm}}$  in the C.M. frame

- Boost the momenta of the two nucleons to lab frame

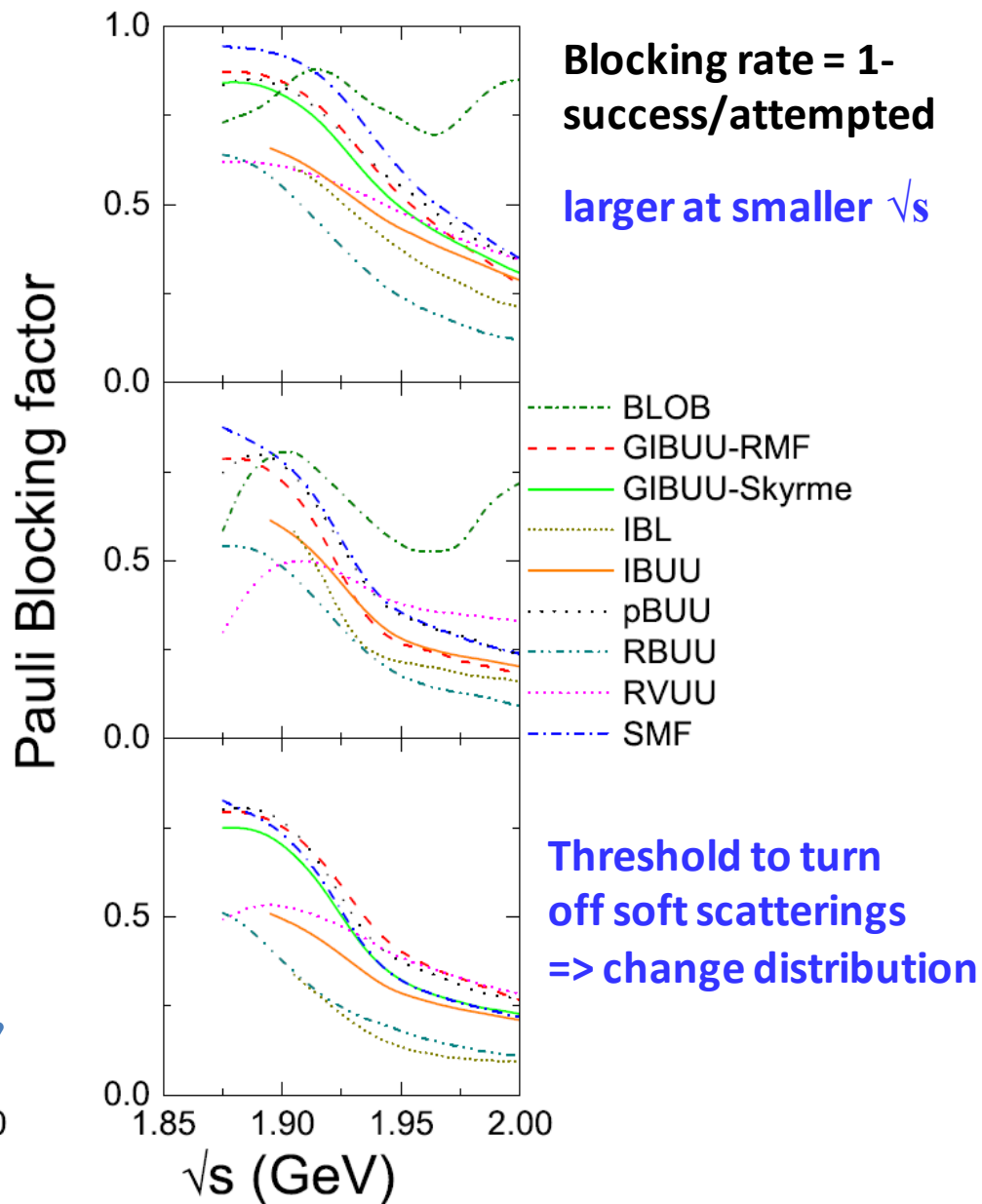
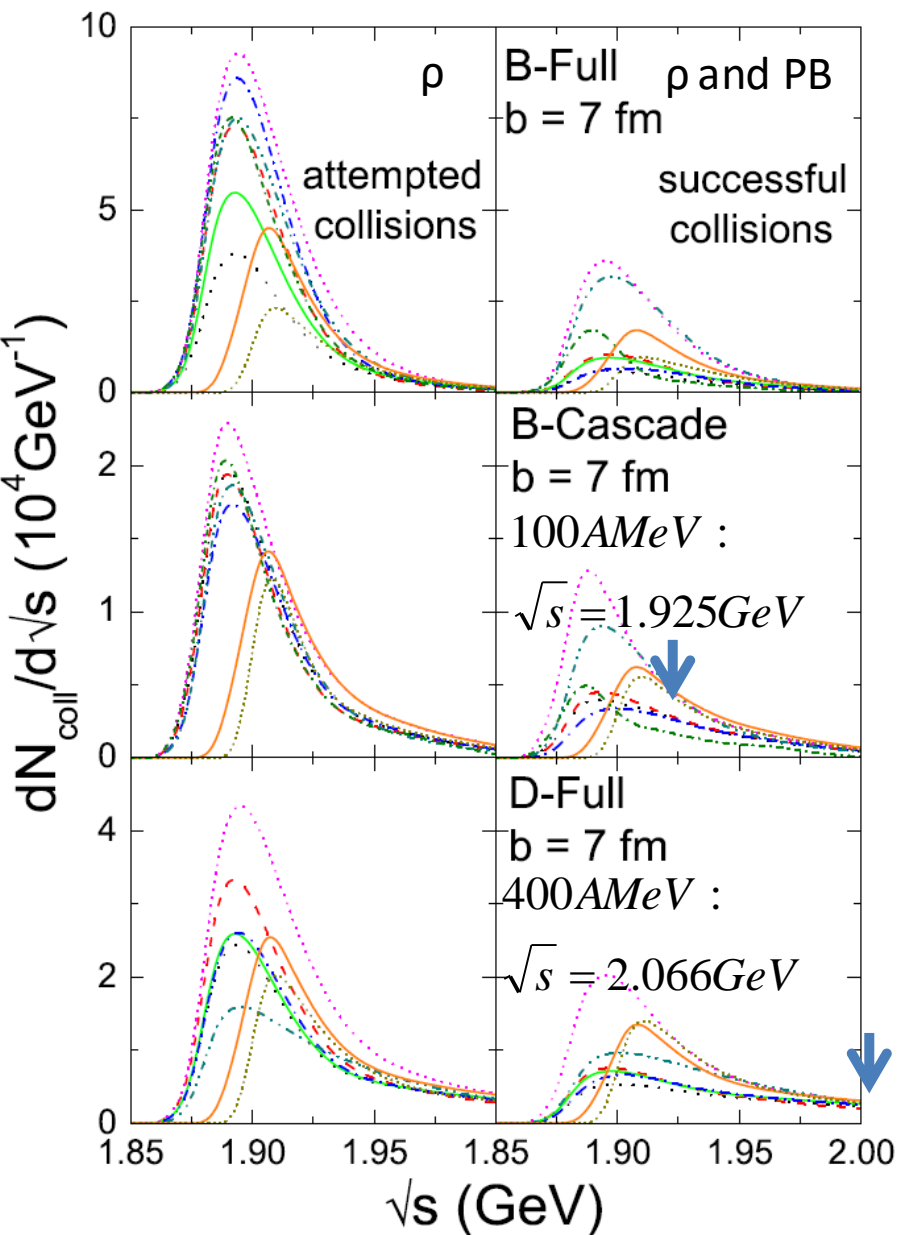
- Check phase space density; if Pauli blocked, return to the initial momenta

# How is Pauli blocking realized?

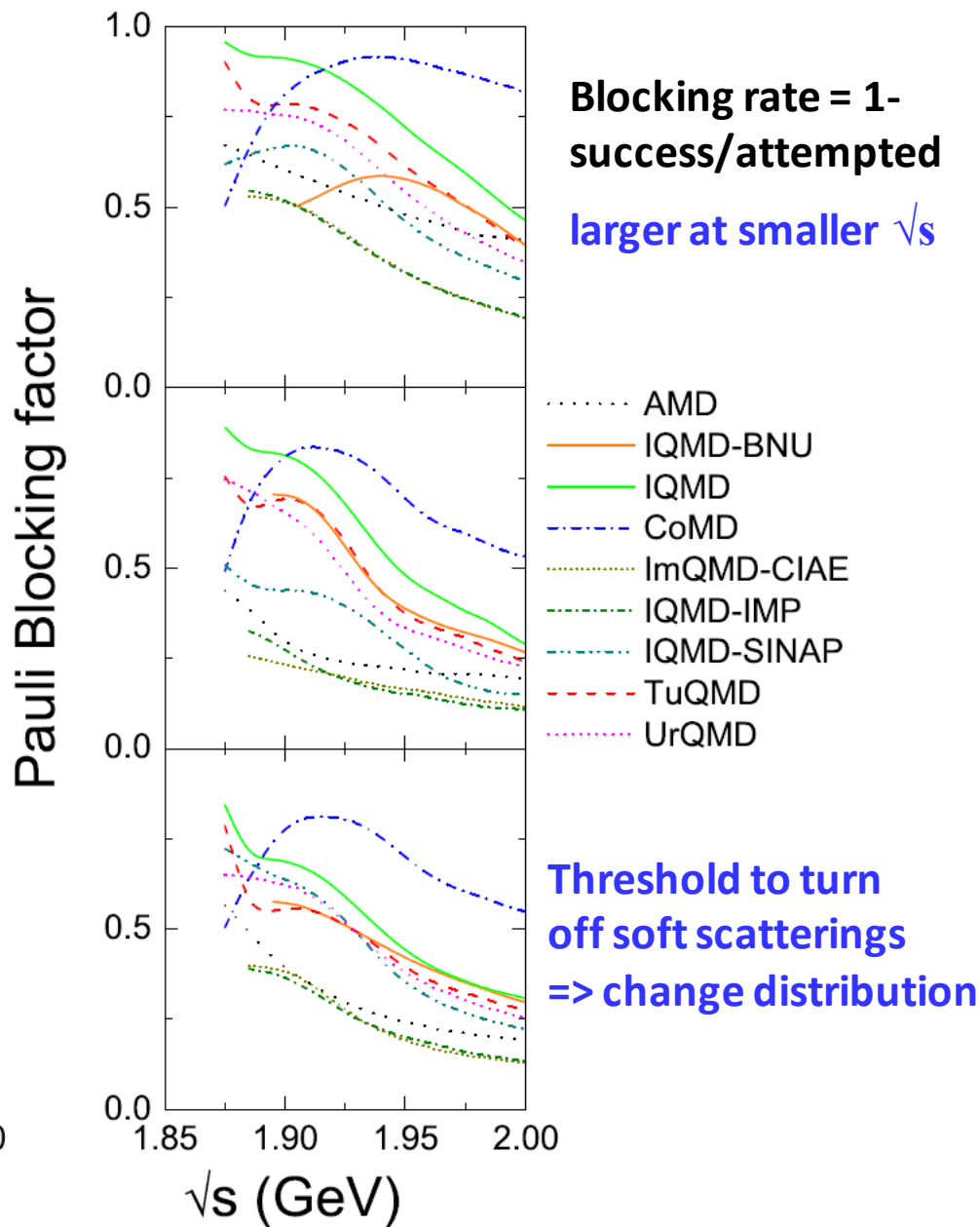
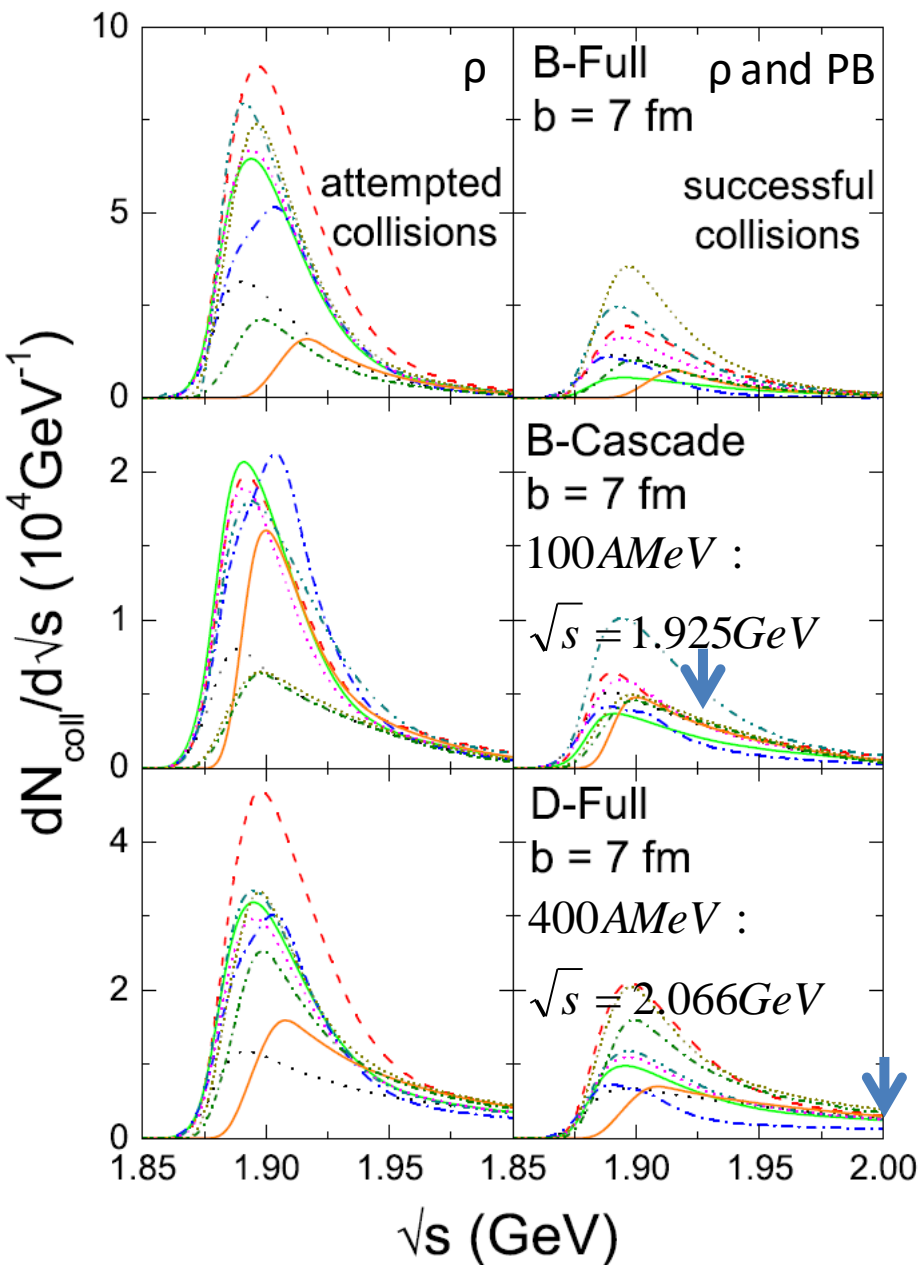
(in most transport models)

- Update the occupation probability  $f_i$  at each time step ( $f_i$  is calculated differently for each code, and can be different for BUU and QMD)
- When a collision is attempted, check the Pauli blocking probability  $1-(1-f_i)(1-f_j)$
- Additional constraint if any (phase-space constraint ...)

# NN scattering & Pauli blocking - BUU



# NN scattering & Pauli Blocking - QMD

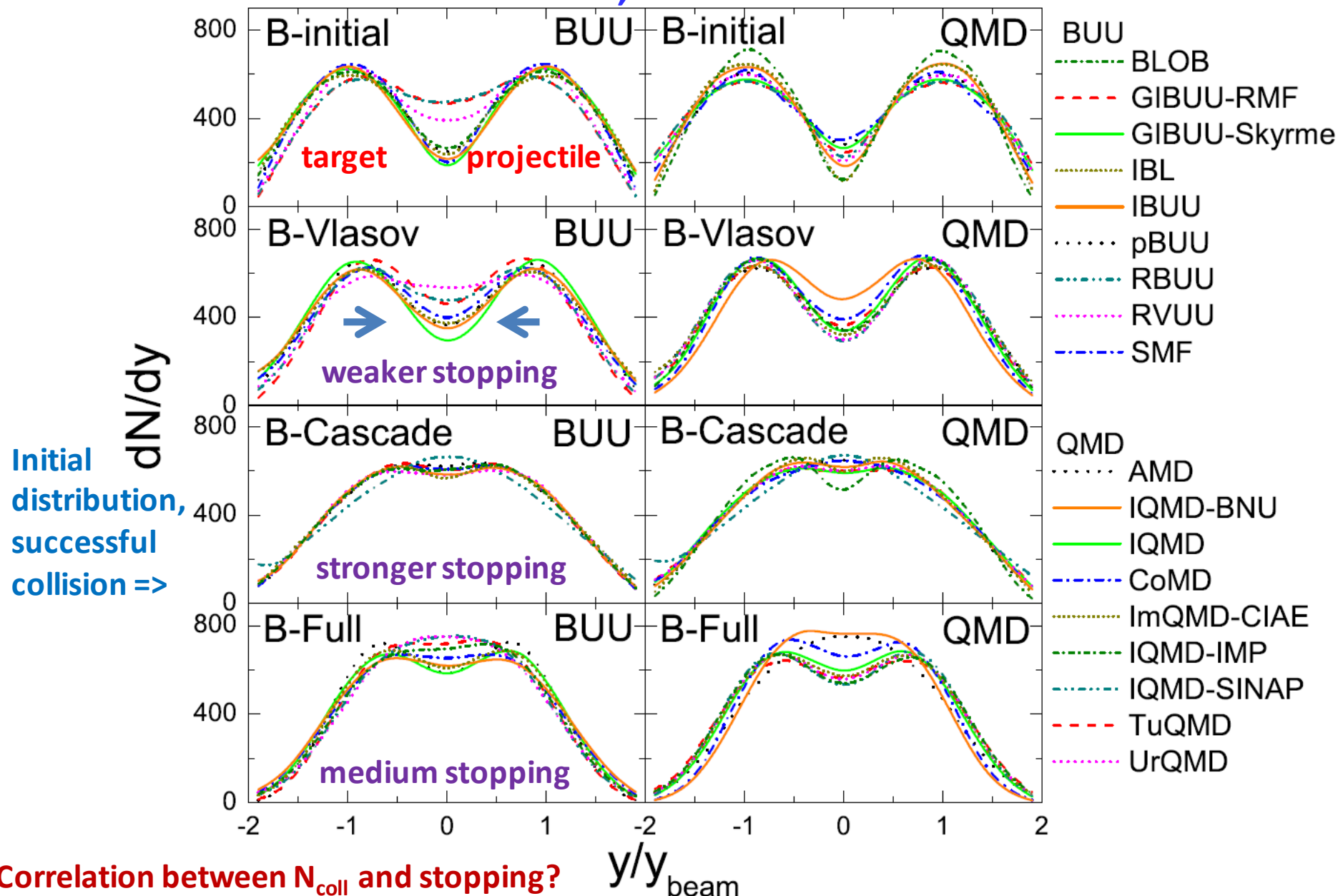


Code name	Occupation probability $f_i$	Blocking probability <sup>a</sup>	Additional constraints
AMD	Antisymmetrized wave packets <sup>b</sup>	Physical wave packet <sup>b</sup>	No
IQMD-BNU	$f_i$ in $h^3$	$1 - (1 - f_i)(1 - f_j)$	Yes <sup>c</sup>
IQMD	$f_i$ in $h^3$	$1 - (1 - f_i)(1 - f_j)$	Yes <sup>d</sup>
CoMD	$f_i$ in $h^3$	$f'_i, f'_j < f_{\max} = 1.05 - 1.1$	Yes <sup>e</sup>
ImQMD-CIAE	$f_i$ in $h^3$	$1 - (1 - f_i)(1 - f_j)$	No
IQMD-IMP	$f_i$ in phase-space cell with $dx = 3.367$ fm, $dp = 89.3$ MeV/ $c$	$1 - (1 - f_i)(1 - f_j)$	No
IQMD-SINAP	$f_i = \sum_k e^{-(\vec{r}_k - \vec{r}_i)^2 / [2(\Delta x)^2]} e^{-(\vec{p}_k - \vec{p}_i)^2 \cdot 2(\Delta x)^2 / \hbar^2}$	$1 - (1 - f_i)(1 - f_j)$	No
TuQMD	$f_i$ in spherical phase-space cell with $dx = 3.0$ fm, $dp = 240$ MeV/ $c$ <sup>f</sup>	$1 - (1 - f_i)(1 - f_j)$	Yes <sup>g</sup>
UrQMD	$f_i = \sum_k e^{-(\vec{r}_k - \vec{r}_i)^2 / [2(\Delta x)^2]} e^{-(\vec{p}_k - \vec{p}_i)^2 \cdot 2(\Delta x)^2 / \hbar^2}$	$1 - (1 - f_i)(1 - f_j)$	Yes <sup>h</sup>
BLOB	$f_i$ in sphere with radius 3.5 fm with Gaussian weight in momentum space <sup>i</sup>	$1 - (1 - f_i)(1 - f_j)$	Yes <sup>j</sup>
GIBUU-RMF	$f_i$ in phase-space cell with $dx = 1.4$ fm, $dp = 68$ MeV/ $c$	$1 - (1 - f_i)(1 - f_j)$	No
GIBUU-Skyrme	$f_i$ in phase-space cell with $dx = 1.4$ fm, $dp = 68$ MeV/ $c$	$1 - (1 - f_i)(1 - f_j)$	No
IBL	$f_i$ in $h^3$	$1 - (1 - f_i)(1 - f_j)$	yes <sup>k</sup>
IBUU	$f_i$ in phase-space cell with $dx = 2.73$ fm, $dp = 187$ MeV/ $c$	$1 - (1 - f_i)(1 - f_j)$	No
pBUU	$f_i$ in same and neighboring spatial cell <sup>l</sup>	$1 - (1 - f_i)(1 - f_j)$	No
RBUU	$f_i$ in phase-space cell with $dx = 1.4$ fm, $dp = 64$ MeV/ $c$	$1 - (1 - f_i)(1 - f_j)$	No
RVUU	$f_i$ in phase-space cell with $dx = 1.14$ fm, $dp = 331$ MeV/ $c$ <sup>m</sup>	$1 - (1 - f_i)(1 - f_j)$	No
SMF	$f_i$ in sphere with radius 2.53 fm with Gaussian weight in momentum space <sup>n</sup>	$1 - (1 - f_i)(1 - f_j)$	No

Code name	Attempted collisions	First collisions within same nucleus	Code name	Attempted collisions	First collisions within same nucleus
AMD	$p = \alpha e^{-\nu R_{ij}^2} v_{ij} \Delta t$	Yes	BLOB	$p = \sigma^{\text{med}} \frac{(\rho_i + \rho_j)}{2} v_{ij} \Delta t$	Yes
IQMD-BNU	Bertsch approach <sup>d</sup>	No	GIBUU-RMF	Bertsch approach	Yes
IQMD	Bertsch approach	Yes	GIBUU-Skyrme	Bertsch approach	Yes
CoMD	$p = 1 - e^{\Delta t / \tau}$	Yes	IBL	Bertsch approach	No
ImQMD-CIAE	Bertsch approach	Yes	IBUU	Bertsch approach	Yes
IQMD-IMP	Bertsch approach	Yes	pBUU	Cell <sup>h</sup>	Yes
IQMD-SINAP	Bertsch approach	Yes	RBUU	Bertsch approach	Yes
TuQMD	Bertsch approach	Yes	RVUU	Bertsch approach	Yes
UrQMD	Collision time table <sup>e</sup>	Yes	SMF	$p = \sigma^{\text{med}} \frac{(\rho_i + \rho_j)}{2} v_{ij} \Delta t$	Yes

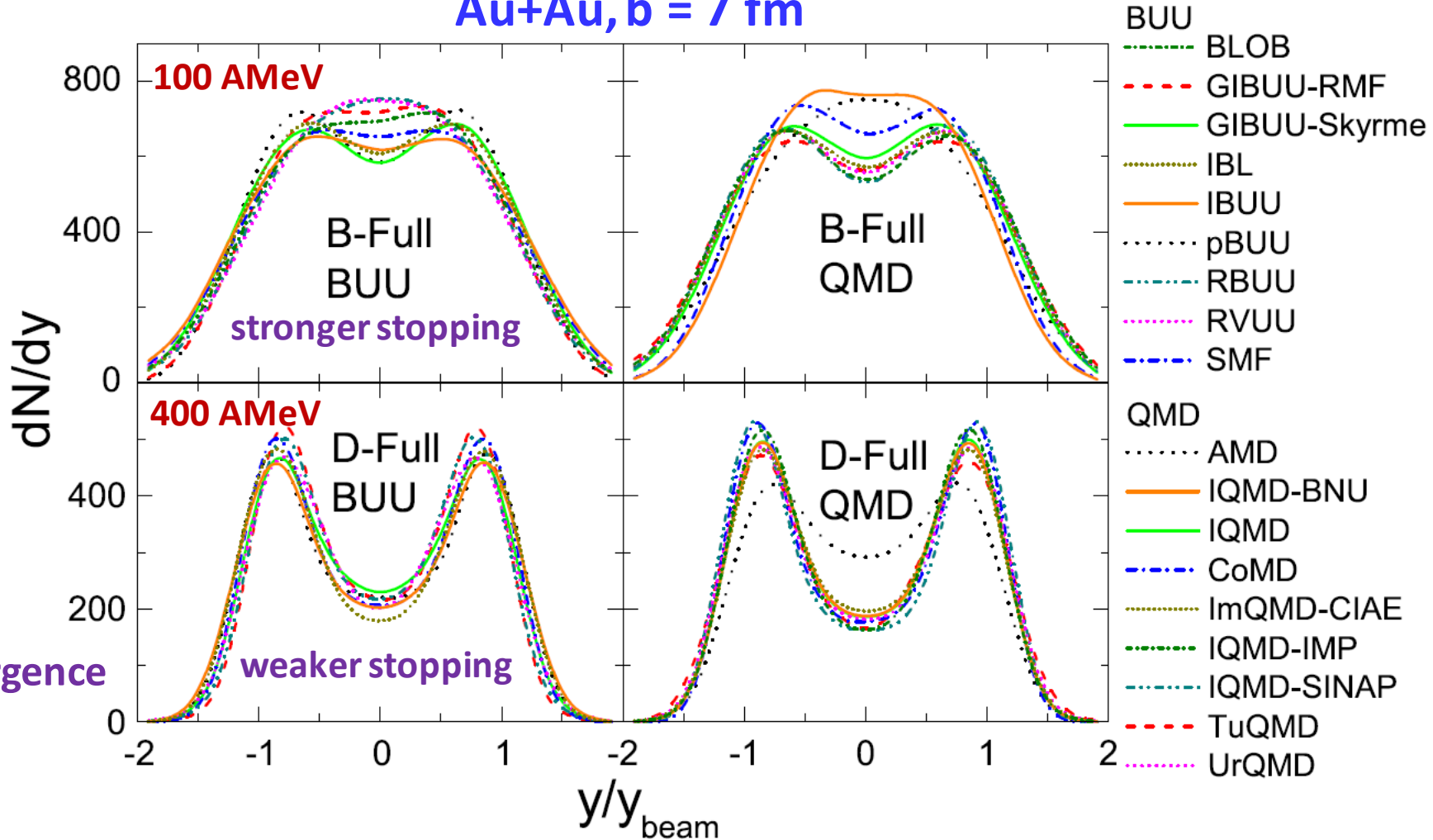
# Rapidity distribution (B-mode)

Au+Au,  $b = 7$  fm



# Rapidity distribution (Full mode)

Au+Au,  $b = 7$  fm

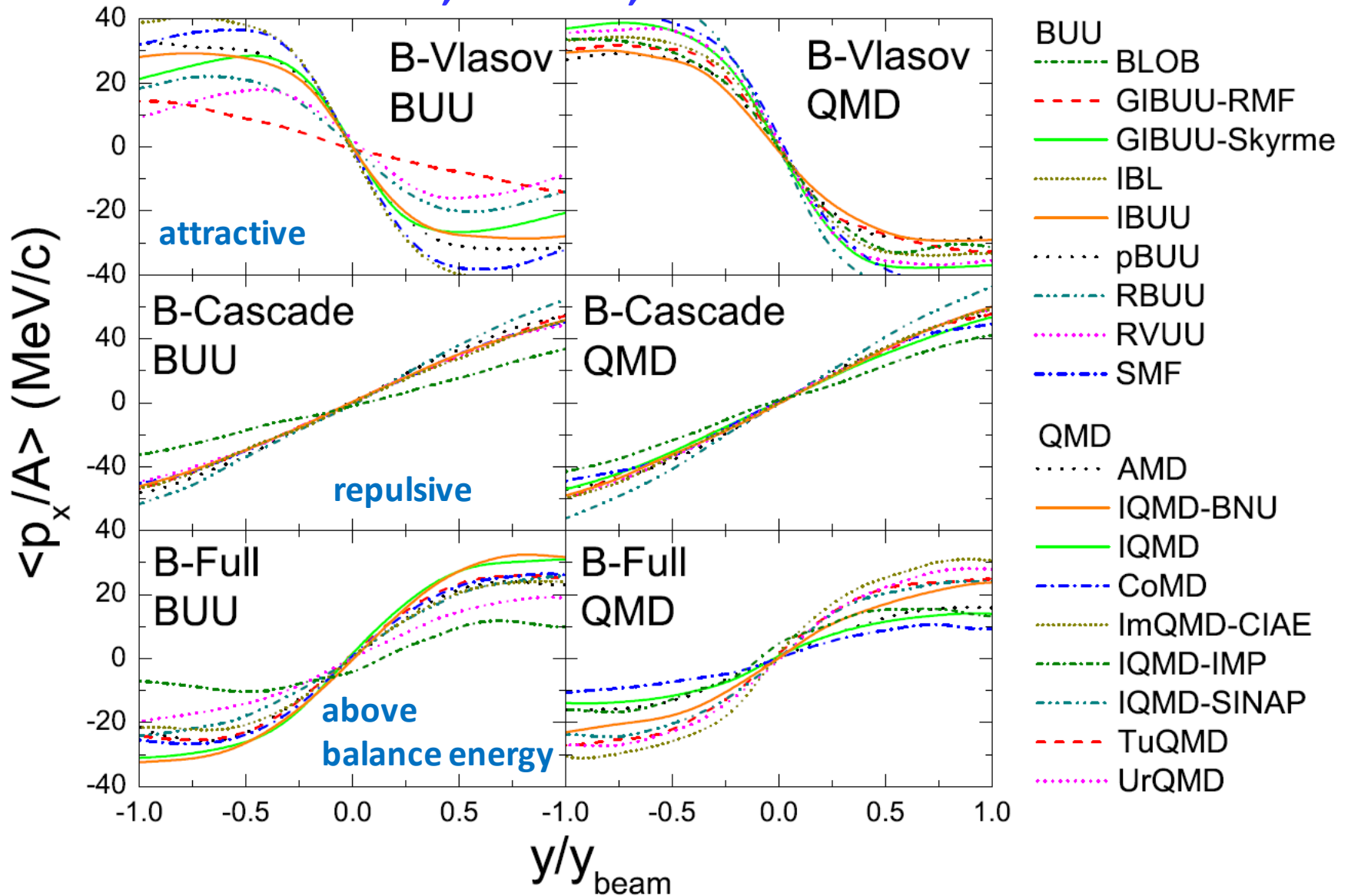


**400 AMeV: weaker Pauli blocking, less sensitive to initialization, good convergence of  $N_{coll}$  at larger  $\sqrt{s}$**



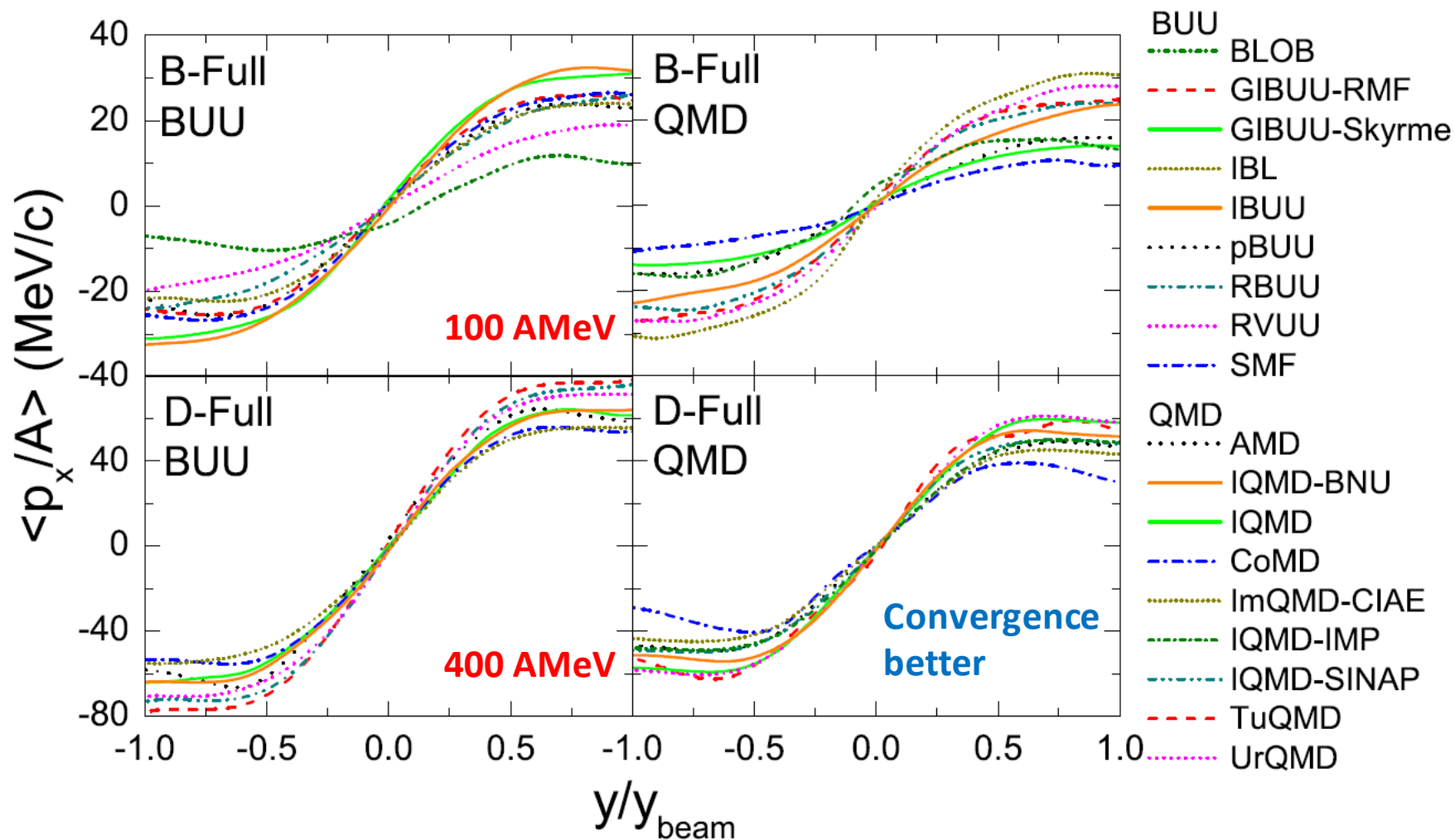
# Transverse flow (B-mode)

Au+Au,  $b = 7$  fm, 100 AMeV

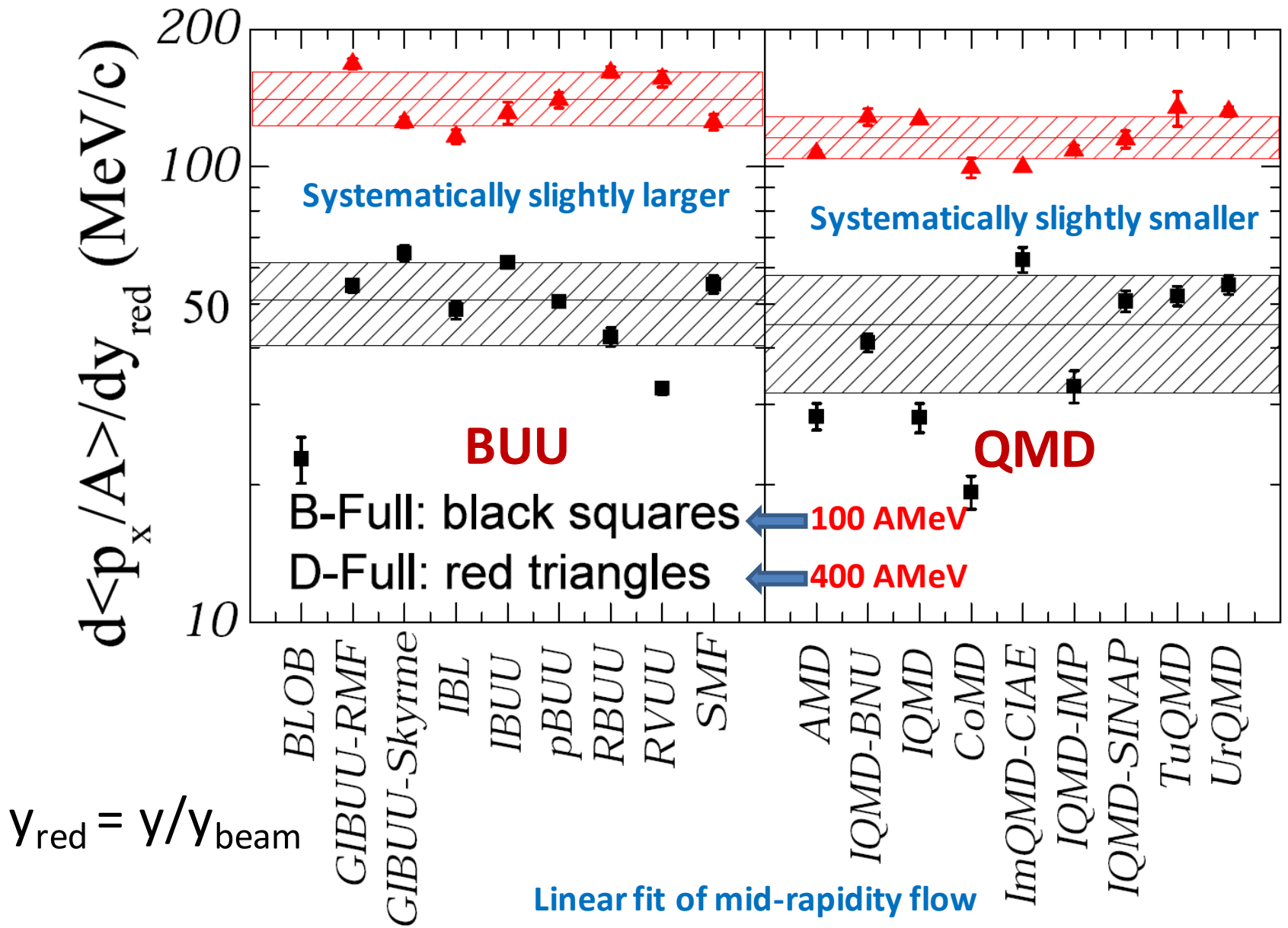


# Transverse flow (Full-mode)

Au+Au,  $b = 7$  fm



Uncertainties: initialization, Pauli blocking



**Theoretical uncertainties of flow parameter:  
about 30% at 100 AMeV, 13% at 400 AMeV**

# conclusions and outlook

- **Initialization** and **Pauli blocking** are the two main sources of uncertainties in heavy-ion simulations
- Theoretically error bar for collective flow is about **13%** at 400 AMeV and **30%** at 100 AMeV (need to be reduced!)
- Future test: **particle production, fluctuation and fragmentation, momentum dependence, ...**

An agreement in treating each part of the simulation

**Towards an accurate description of heavy-ion collisions!**

# Transport2016 - box calculation

## the Box Simulation Organizing Committee

Maria Colonna

Akira Ono

Yongjia Wang

Jun Xu

Yingxun Zhang

**Initial configuration well controlled**

**Theoretical answer available**

**collision rate, blocking rate, mean field**

## Local organizers:

**Chair:** Fengshou Zhang (BNU, China)

Lie-Wen Chen (SJTU, China), Qingfeng Li (HZU, China), Yongjia Wang (HZU, China), Jun Xu (SINAP, China), Yingxun Zhang (CIAE, China), Zhigang Xiao (TSHU, China), Fengshou Zhang (BNU, China)

**Date: June 18th, 2016, right after Nusym16**

<http://info.phys.tsinghua.edu.cn/enpg/nusym16/htmls/transport-model.html>

*Thank you!*

**xujun@sinap.ac.cn**