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Comparison of heavy-ion transport simulations: Collision integral in a box

Yingxun Zhang (张英逊)
China Institute if Atomic Energy

Yongjia Wang, Maria Colonna, Pawel Danielewicz, Akira Ono, Betty Tsang, Hermann Wolter, Jun Xu,
Lie-Wen Chen, Dan Cozma, Zhao-Qing Feng, Che-Ming Ko, Bao-An Li, Qing-Feng Li, S. Das Gupta, N. Ikeno, C.M. Ko, B.A.Li, Q.F.Li, Z.X. Li, S. Mallik, T. Ogawa, D. Oliinychenko, M. Papa, H. Petersen, Jun Su, Taesoo Song, Janus Weil, Ning Wang, Feng-Shou Zhang, Guo-Qiang Zhang, and Zhen Zhang,
……..

Hermann is working on the transport paper

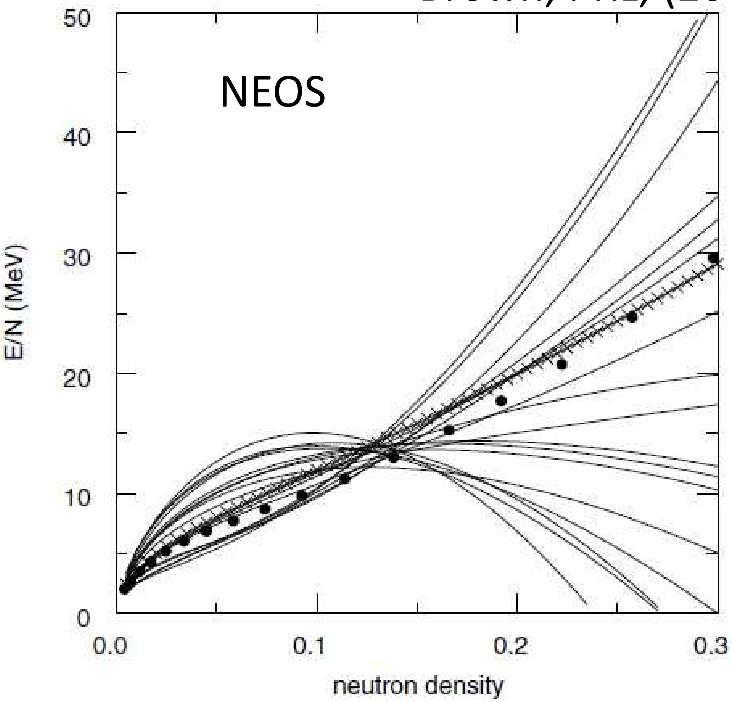
Isospin asymmetric Equation of State

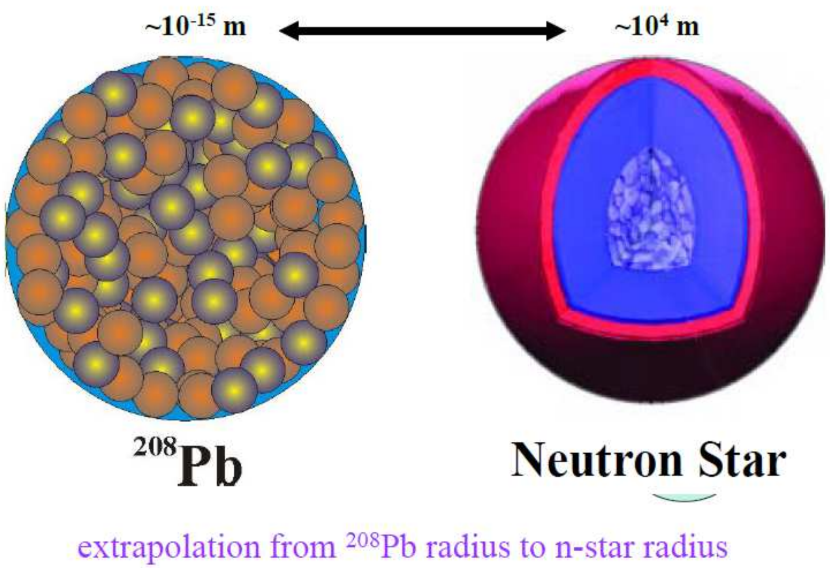
$$E(\rho,\delta) = E(\rho,\delta=0) + S(\rho)\delta^2 + O(\delta^4)$$

It is a fundamental properties of nuclear matter, and is very important for understanding

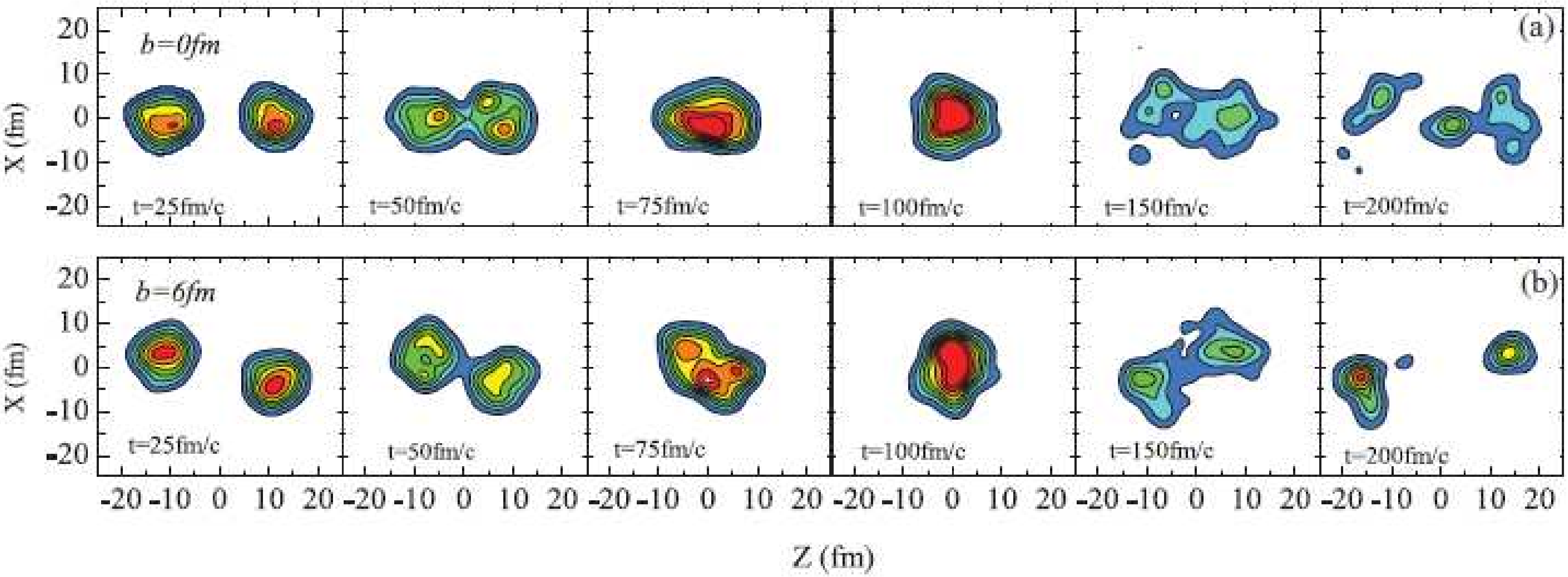
- *properties of nuclear structure*
- *properties of neutron star*
- *properties of heavy ion reaction mechanism*

Brown, PRL, (2000)



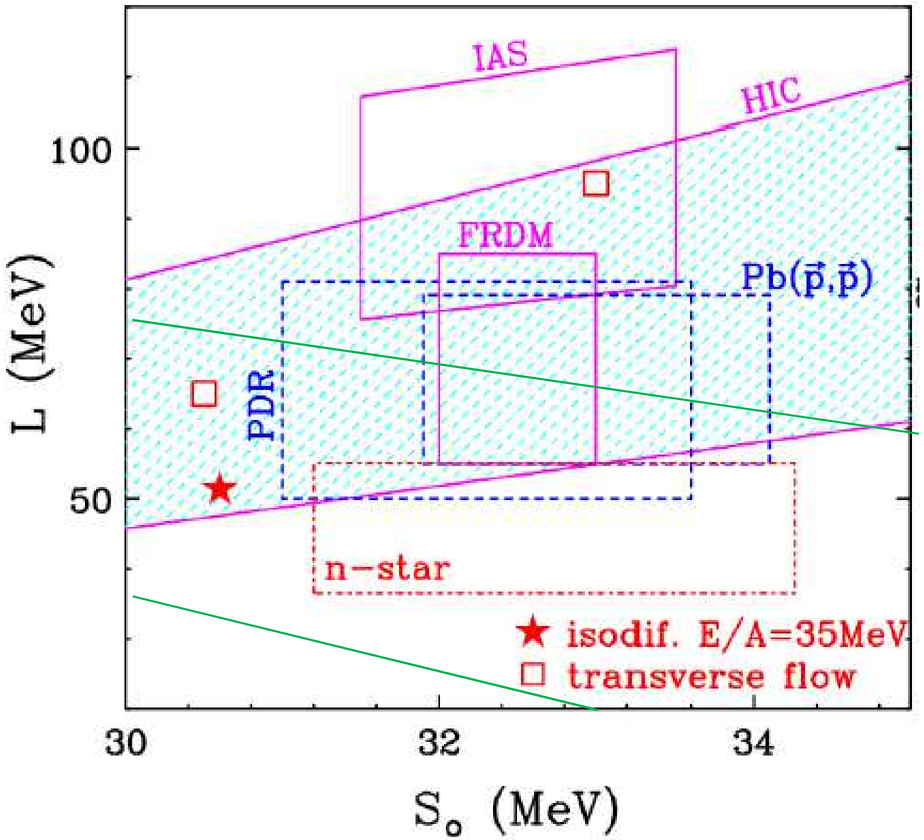


C.J. Horowitz, J. Piekarewicz, Phys. Rev. Lett. 86 (2001) 5647



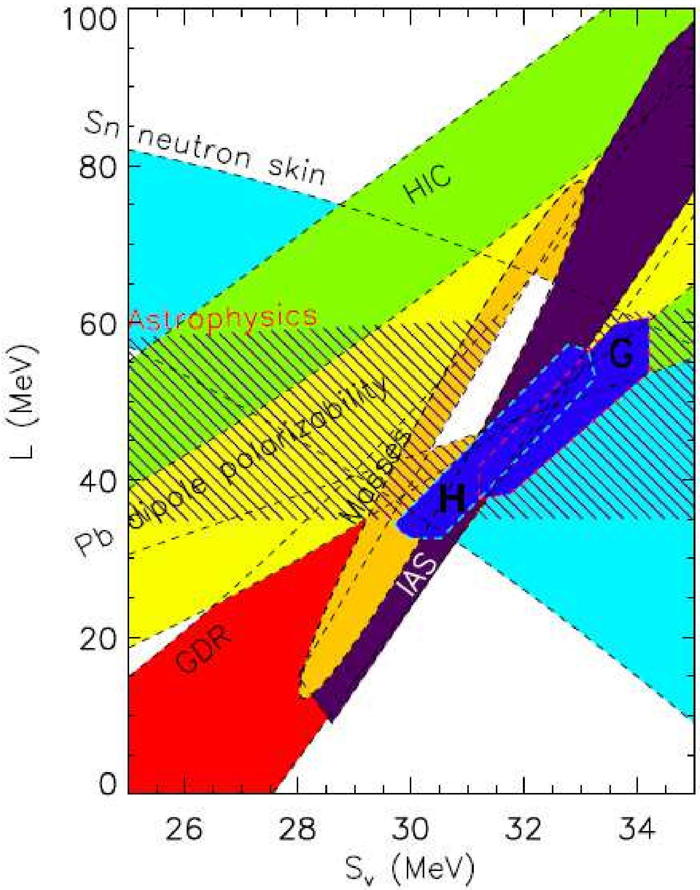
Probing the Equation of State via Heavy ion collisions

M.B.Tsang, Yingxun Zhang, et.al., PRL2009

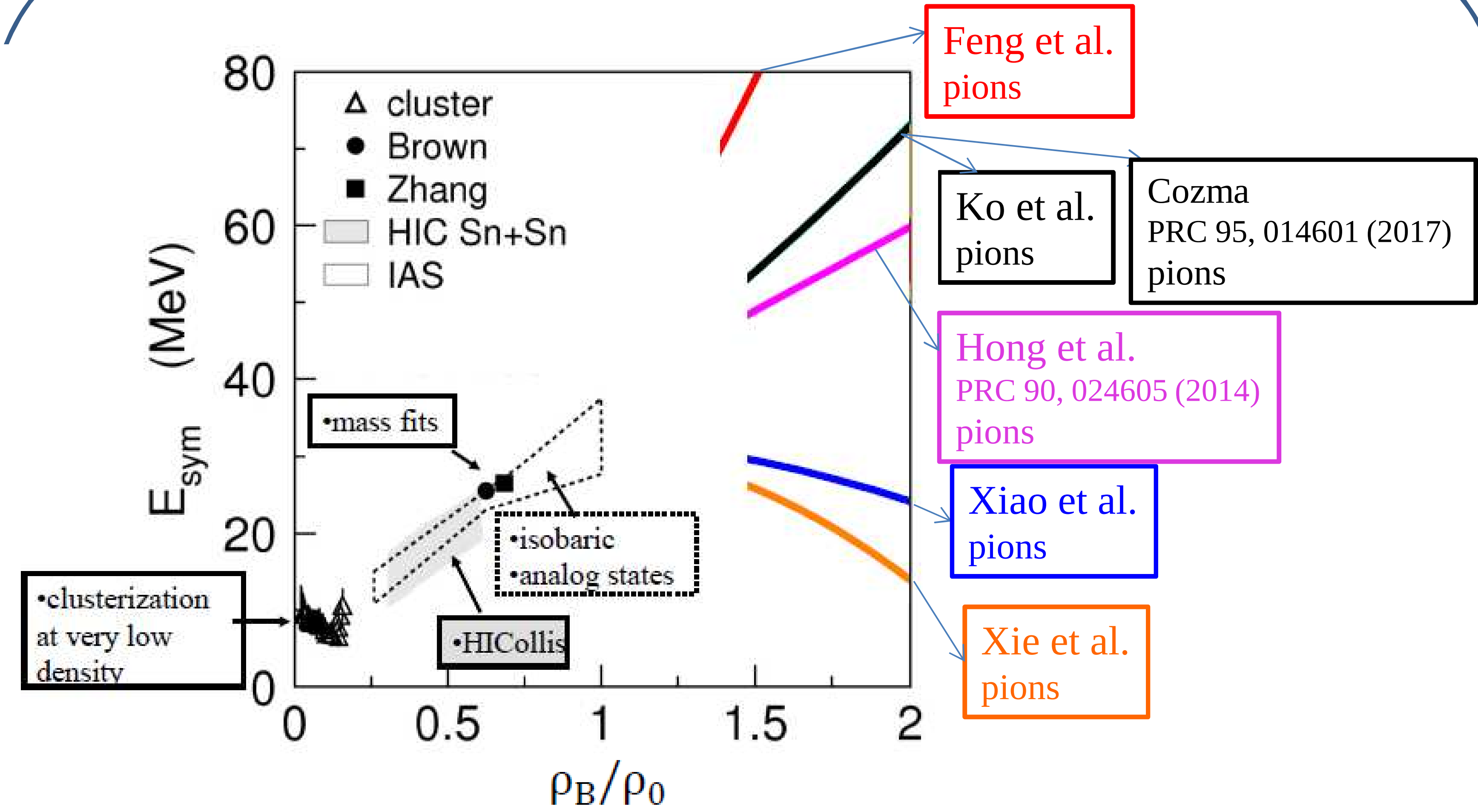


$$S(\rho) = S_0 + \frac{L}{3}\left(\frac{\rho - \rho_o}{\rho_o}\right) + \frac{K_{\text{sym}}}{18}\left(\frac{\rho - \rho_o}{\rho_o}\right)^2 + \ldots,$$

Lattimer, EPJA 50 (2014) 40



Constraints on the symmetry energy at suprasaturation density



Constraints on symmetry energy depends on the transport code !

Why the conclusions are different from different transport codes?

1, Different physics inputs

- mean field potential,
- in-medium n-n cross section,
- initial density distribution,
- ……

2, Different technical assumption for solving the transport equation

- BUU, QMD, shape of t.p., full/parallel ensemble, ……

Systematic comparison of transport codes under the control condition

Efforts on this direction, since 2004, 2009, 2014, 2015,2016, ….

Transport 2014, Shanghai

Writing group
J. Xu
L.W. Chen
B. Tsang
H. Wolter
Y.X. Zhang

Transport Code Comparison Project

Boltzmann-like (9)

	Code Name	Who did?
1	BLOB	P. Napolitani
2	SMF	M. Colonna
3	GiBUU(Sky)	J. Weil/U. Mosel
4	GiBUU(RMF)	J. Weil
5	RVUU	Taesoo Song
6	IBUU(04)	Jun Xu
7	IBL	Wen-Jie Xie
8	RBUU	Kyungil Kim
9	pBUU	P. Danielewicz

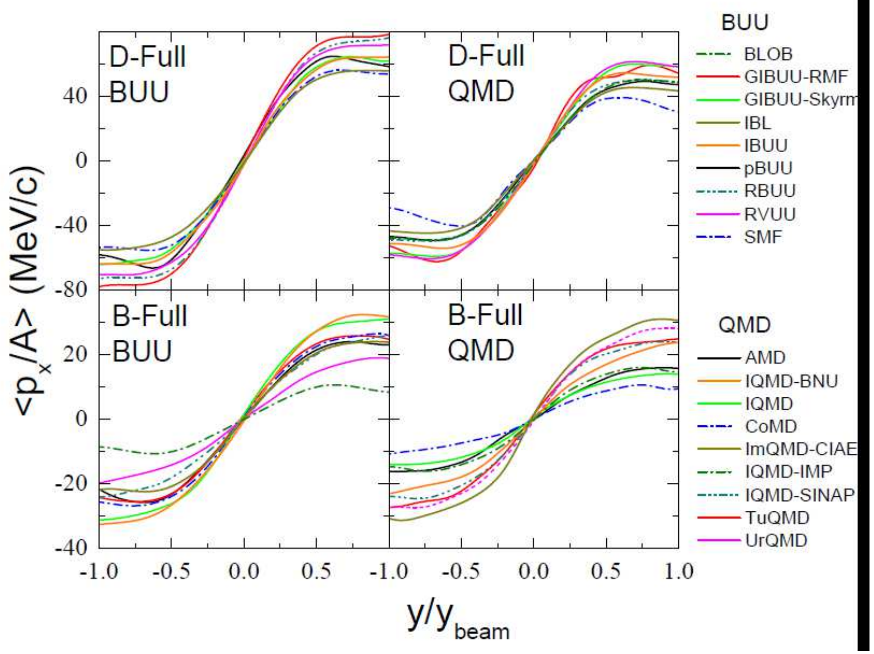
MD-like (9)

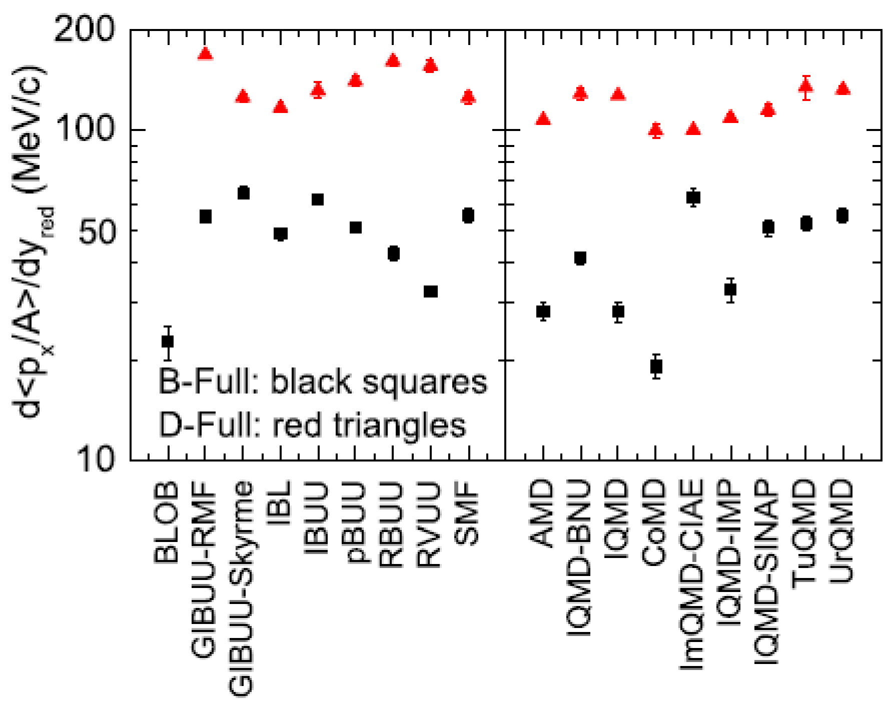
	Code Name	Who did?
1	AMD	Akira Ono
2	CoMD	Maximo Papa
3	ImQMD-CIAE	Ying-Xun Zhang
4	IQMD	Ch. Hartnack
5	IQMD-BNU	Jun Su
6	IQMD-SINAP-	Guo-Qiang Zhang
7	LQMD-IMP	Zhao-Qing Feng
8	UrQMD (L=1)	Yong-Jia Wang
9	TuQMD	Dan Cozma

PHYSICAL REVIEW C 93, 044609 (2016)

Understanding transport simulations of heavy-ion collisions at 100A and 400A MeV: Comparison of heavy-ion transport codes under controlled conditions

Jun Xu,[1,*] Lie-Wen Chen,[2,†] ManYee Betty Tsang,[3,‡] Hermann Wolter,[4,§] Ying-Xun Zhang,[5,‖] Joerg Aichelin,[6] Maria Colonna,[7] Dan Cozma,[8] Pawel Danielewicz,[3] Zhao-Qing Feng,[9] Arnaud Le Fèvre,[10] Theodoros Gaitanos,[11] Christoph Hartnack,[6] Kyungil Kim,[12] Youngman Kim,[12] Che-Ming Ko,[13] Bao-An Li,[14] Qing-Feng Li,[15] Zhu-Xia Li,[5] Paolo Napolitani,[16] Akira Ono,[17] Massimo Papa,[18] Taesoo Song,[19] Jun Su,[20] Jun-Long Tian,[21] Ning Wang,[22] Yong-Jia Wang,[15] Janus Weil,[19] Wen-Jie Xie,[23] Feng-Shou Zhang,[24] and Guo-Qiang Zhang[1]





In the simulations of HICs

- Initial conditions are hard to control
- there is no theoretical results to benchmark the codes

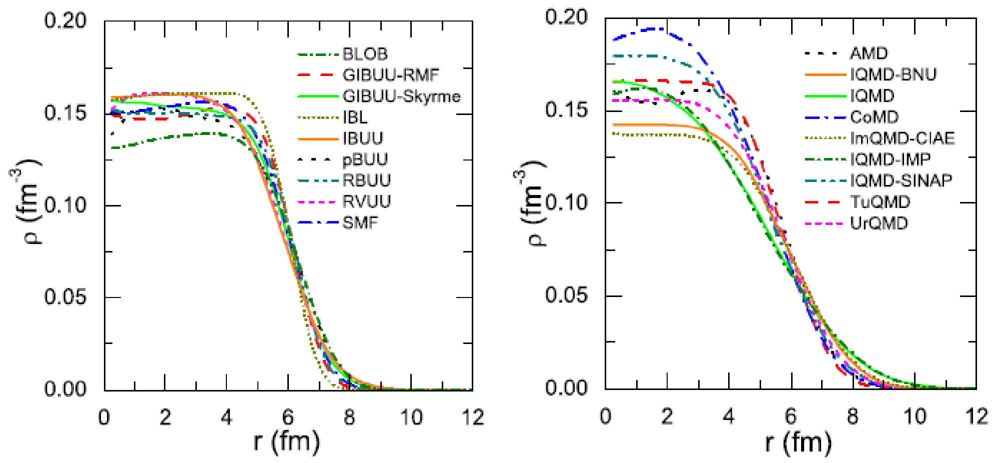
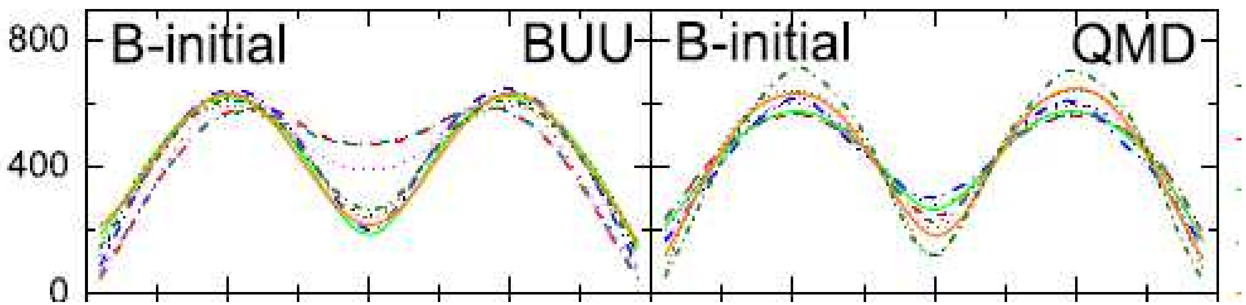


FIG. 1. Initial density profiles for BUU-type (left) and QMD-type (right) models.



Design the BOX simulations Homework

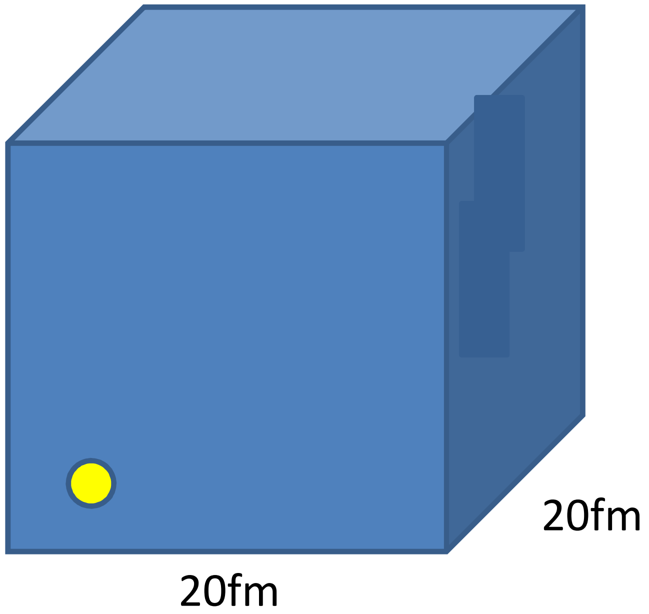
Advantages in BOX simulations

- Initial conditions are straightforward to realize,
- We can test collision and mean field part separately
- there are some exact limits available from kinetic theory or Landau theory,

Keep in mind:

- Fundamental differences may be present between an idealized kinetic equation and a simulation,
- One cannot expect BUU and QMD completely agree with each other,

- The box calculations are performed with **periodic boundary conditions (BC)**.



•Details of periodic boundary conditions

1. a box of volume $V = L_1 * L_2 * L_3$, where the system is confined.

2. The position of the center of box is $(L_1/2, L_2/2, L_3/2)$.

3. In order to keep all particles inside the box, a particle leaving the box has to enter it on the opposite side, keeping the same momentum.

HW2, RVUU: -10, 10 fm, GiBUU: -10, 10fm, UrQMD:-10:10fm

Homework 1 (Cascade mode) in BOX simulations

Initialization:

- **Uniform density ρ_0=0.16 fm^{-3}**
- A=1280, n=p=640
- Particle positions are initialized randomly from 0 to L_k.
- **Particle momenta are initialized randomly in a sphere with Fermi momentum p_F=265 MeV/c for T=0 case, or with the Fermi distribution at T=5MeV**

Cross section

- **constant isotropic elastic cross section of \sigma=40 mb**

The simulation should be followed until t=140 fm/c, with a recommended step of Dt=0.5 or 1.0 fm/c.

6 calculations: 3 modes (C,CBOP1, CBOP2), and 2 temperatures (T0,T5).

	Collision without PB	Collision with PB_op1 (same in HIC)	Collision with PB_op2 (f_i=Fermi-Dirac)
T=0MeV	CT0	CBop1T0	CBOP2T0
T=5MeV	CT5	CBop1T5	CBOP2T5

16 transport codes in comparison with BOX condition

	BUU-type	Contributor		QMD-type	
1	BUU-VM	S. Mallik	1	CoMD	M. Papa
2	GiBUU	J. Weil	2	ImQMD	Y.X.Zhang, Z.X. Li
3	IBUU	Ju Xu, L.W.Chen, B.A.Li	3	IQMD-BNU	J.Su, F.S.Zhang
4	pBUU	P. Danielewicz	4	IQMD-IMP	Z.Q.Feng
5	RVUU	T. Song, Z. Zhen, C.M. Ko	5	IQMD-SINAP	G.Q.Zhang
6	SMF	M.Colonna	6	JAM	A.Ono, N.Ikeno, Y.Nara
7	SMASH	D. Oliinychenko	7	JQMD	T. Ogawa
			8	TuQMD	D. Cozma
			9	UrQMD	Y.J.Wang, Q.F.Li

Results without Pauli-Blocking

A. Exact limits of collision rates

$$\frac{\mathrm{d}N_{\mathrm{coll}}}{\mathrm{d}t} = \frac{A}{2\rho}\, g^2 \int \frac{\mathrm{d}^3p\, \mathrm{d}^3p_1}{(2\pi\hbar)^6}\, v_{\mathrm{rel}}\, \sigma^{\mathrm{med}}\, f(p)\, f(p_1)$$

$$= \frac{1}{2} A\, \rho\, \langle v_{\mathrm{rel}}\, \sigma^{\mathrm{med}} \rangle\, .$$

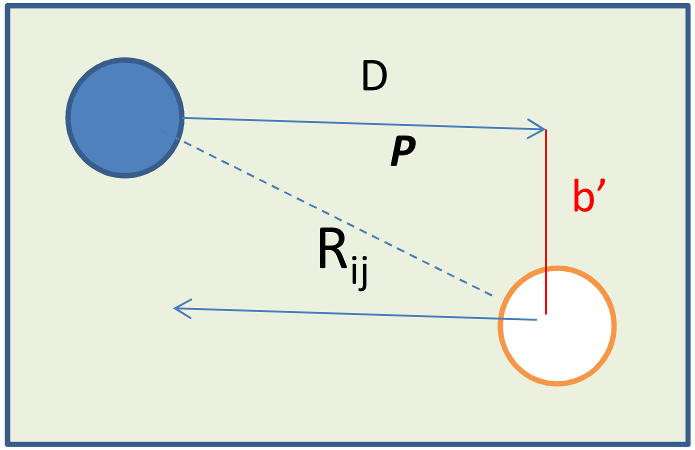
Non-relativistic

		Fermi		Boltzmann	
		$T=0$	$T=5$ MeV	$T=0$	$T=5$ MeV
Non-relativistic	Num. Int.	118.1 [a]	122.1	115.9 [a]	120.1
	Cascade	118.2	122.1	115.9	120.1
Quasi-relativistic	Num. Int.	115.0	118.8	112.3	116.3
	Cascade	115.0	118.8	112.3	116.3
Relativistic	Num. Int.			111.4	115.4
	Cascade ($\delta t = \alpha\Delta t$)	114.0	117.8	111.4	115.4
	Cascade ($\delta t = \Delta t$)	115.2	119.0	112.7	116.7

Collision criterion

Type A: Closest distance approach

- In two particle c.m.



$$b < \sqrt{\sigma^{\mathrm{med}}/\pi}$$

$$\left|\frac{\Delta \boldsymbol{r}\cdot\boldsymbol{p}}{p}\right| < \left(\frac{p}{\sqrt{p^2+m_1^2}} + \frac{p}{\sqrt{p^2+m_2^2}}\right)\delta t/2$$

$$\boldsymbol{\beta} = (\boldsymbol{p}_1 + \boldsymbol{p}_2)/(E_1 + E_2)$$

$$\boldsymbol{p} = \gamma\left(\frac{\boldsymbol{p}_1\cdot\boldsymbol{\beta}}{\beta} - \beta E_1\right)\frac{\boldsymbol{\beta}}{\beta} + \left(\boldsymbol{p}_1 - \frac{\boldsymbol{p}_1\cdot\boldsymbol{\beta}}{\beta}\frac{\boldsymbol{\beta}}{\beta}\right)$$

$$\Delta\boldsymbol{r} = (\gamma - 1)\{(\boldsymbol{r}_1 - \boldsymbol{r}_2)\cdot\boldsymbol{\beta}/\beta\}\boldsymbol{\beta}/\beta + (\boldsymbol{r}_1 - \boldsymbol{r}_2)$$

- Computational frame

$$\delta t = \alpha \Delta t$$

$$\alpha = \gamma\frac{E_1^* E_2^*}{E_1 E_2}$$

Type B: probability of binary collision

$$\xi < \underline{P = \frac{1}{2}\sigma v_{ij}\rho_i \Delta t}$$ SMF

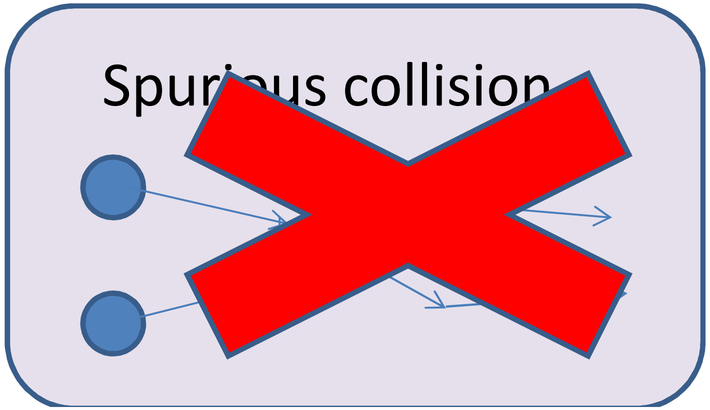
$$\overline{P = 1 - e^{-\sigma v_{ij}\rho_i \Delta t}}$$ CoMD

$$P = \frac{\sigma}{N_{\mathrm{TP}}}\frac{1}{\gamma V_{\mathrm{cell}}} v_{ij}^{*} \alpha \Delta t$$ pBUU

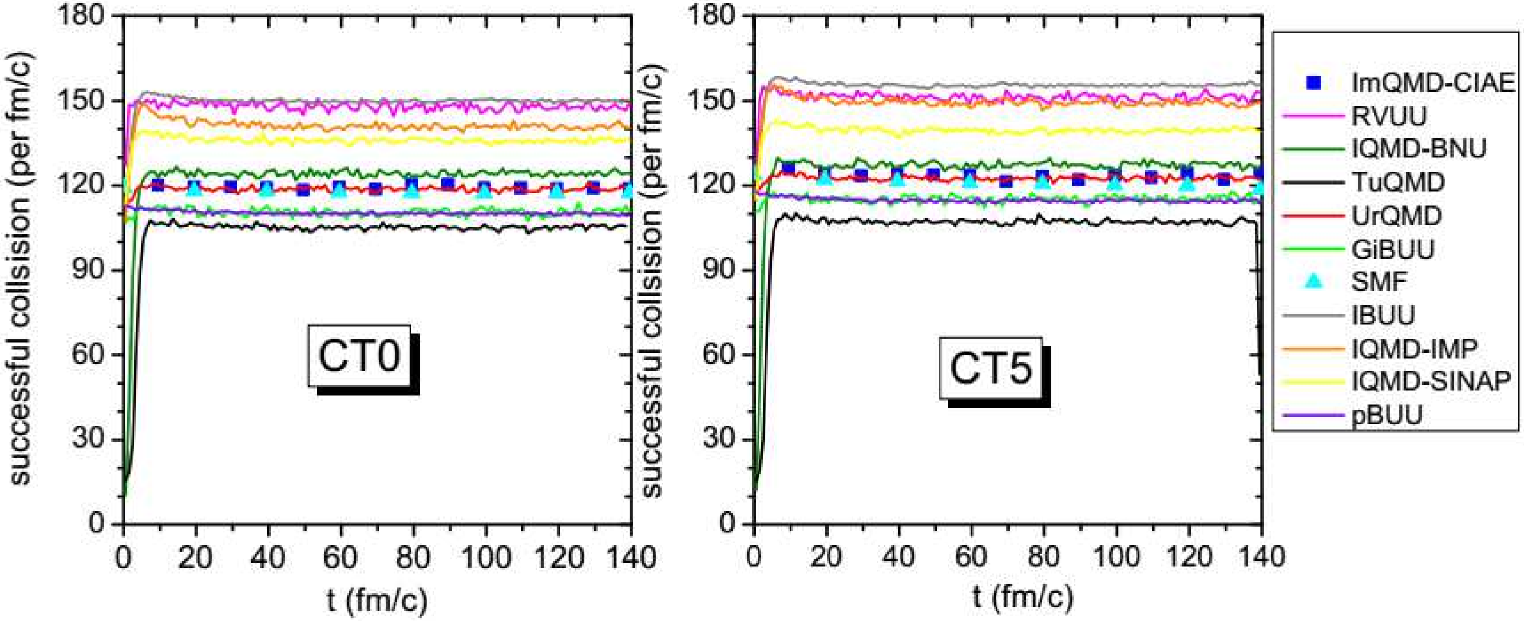
TABLE IV: Characteristics of collision procedures in different codes and a simple cascade code. The notation "$P = x$" stands for a condition that is satisfied randomly with the probability x. Comma-separated conditions stand for the logical conjunction.

BUU-type	Distance condition	Time condition	Collision order
BUU-VM	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
GiBUU	$\pi d_\perp^{*2} < \sigma/N_{\rm TP}$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
IBUU	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
pBUU	$i, j \in$ the same $V_{\rm cell}$ volume	$P = \frac{\sigma}{N_{\rm TP}} \frac{1}{\gamma V_{\rm coll}} v^*_{ij} \alpha \Delta t$	randomly nominate (i, j) pairs
RVUU	$\pi d_\perp^{*2} < \sigma_{\rm max}/N_{\rm TP}$, $P = \sigma/\sigma_{\rm max}$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
SMASH	$\pi d_\perp^{*2} < \sigma/N_{\rm TP}$	$t^{(\rm ref)}_{\rm coll} \in [t_0,\ t_0 + \Delta t]$	ordered by $t^{(\rm ref)}_{\rm coll}$
SMF	$j =$ closest to i in same ensemble	$P = \frac{1}{2}\sigma v_{ij}\rho_i \Delta t$	cyclic with random starting for i
QMD-type	**Distance condition**	**Time condition**	**Collision order**
CoMD	$j =$ closest to i, $j > i$ [a]	$P = 1 - e^{-\sigma v_{ij}\rho_i \Delta t}$	cyclic with random starting for i
ImQMD	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\gamma\Delta t$	fixed order
IQMD-BNU	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
IQMD-IMP	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\gamma\Delta t$	fixed order
IQMD-SINAP	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\gamma\Delta t$	fixed order
JAM	$\pi d_\perp^{*2} < \sigma$	$\bar{t}_{\rm coll} \in [t_0,\ t_0 + \Delta t]$	ordered by $\bar{t}_{\rm coll}$
JQMD	$d^*_\perp < b_{\rm max}$, $P = \sigma/\pi b^2_{\rm max}$	$\lvert \bar{t}_{\rm coll} - t_0\rvert < \frac{1}{2}\Delta t$	fixed order
TuQMD	$\pi d_\perp^{*2} < \sigma$	$t^*_{1-}, t^*_{2-} < t^*_{\rm coll} < t^*_{1+}, t^*_{2+}$	randomly ordered
UrQMD	$\pi d_\perp^{*2} < \sigma$	$t^{(\rm ref)}_{\rm coll} \in [t_0,\ t_0 + \Delta t]$	ordered by $t^{(\rm ref)}_{\rm coll}$
Simple Cascade	**Distance condition**	**Time condition**	**Collision order**
rel.($\delta t = \alpha\Delta t$)	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\alpha\Delta t$	fixed order
rel.($\delta t = \Delta t$)	$\pi d_\perp^{*2} < \sigma$	$\lvert t^*_{\rm coll} - t^*_0\rvert < \frac{1}{2}\Delta t$	fixed order
quasi-relativistic	$\pi d_\perp^{(\rm ref)2} < \sigma$	$\lvert t^{(\rm ref)}_{\rm coll} - t_0\rvert < \frac{1}{2}\Delta t$	fixed order

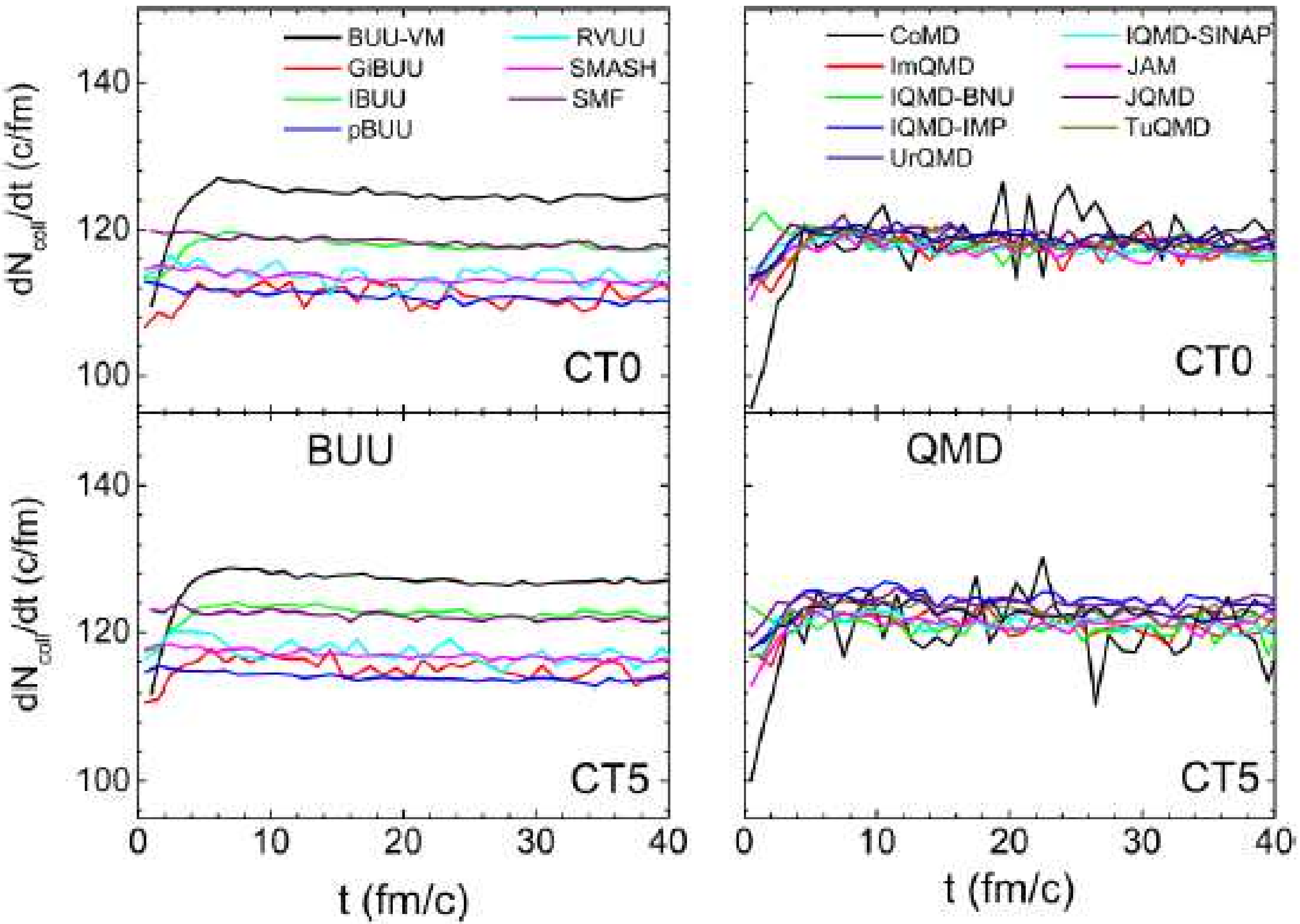
The way on determining the collision in closest distance approach, does not preclude the spurious collisions



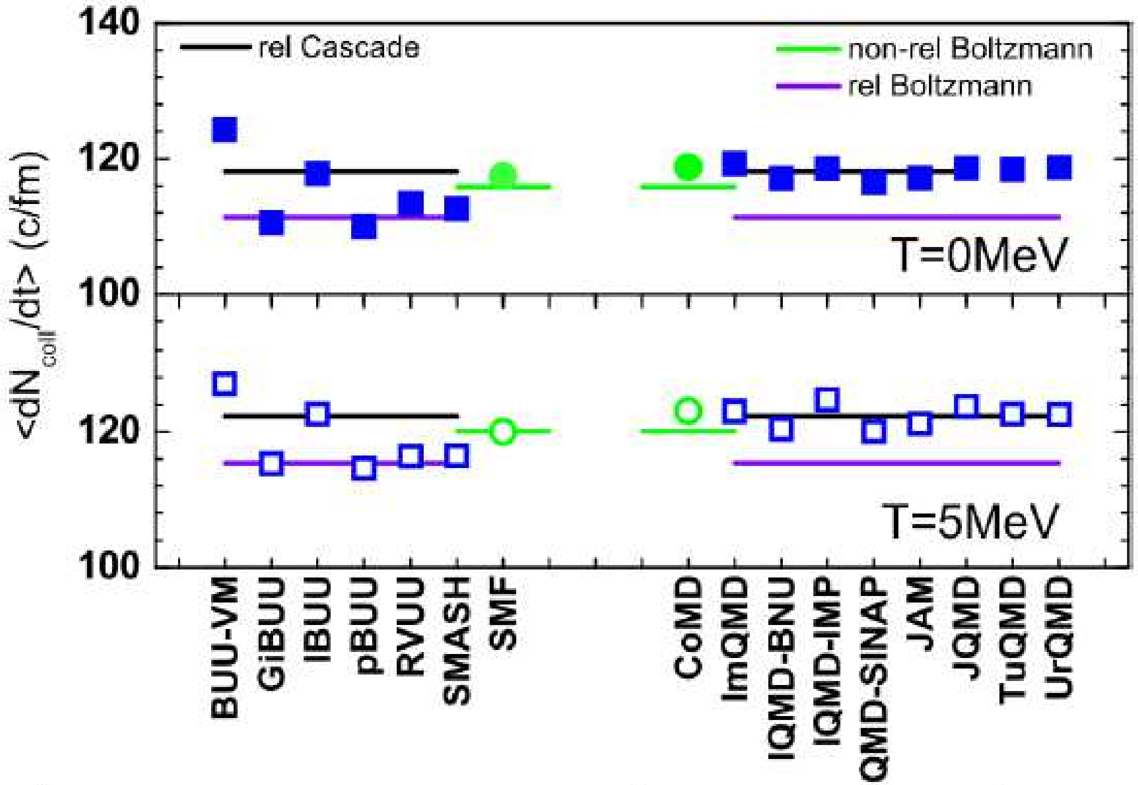
With spurious collisions, collision rate is up to 150-170c/fm

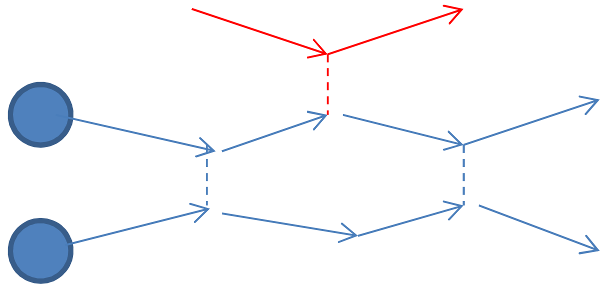


Results of without Pauli blocking



Independent of time interval in simulations





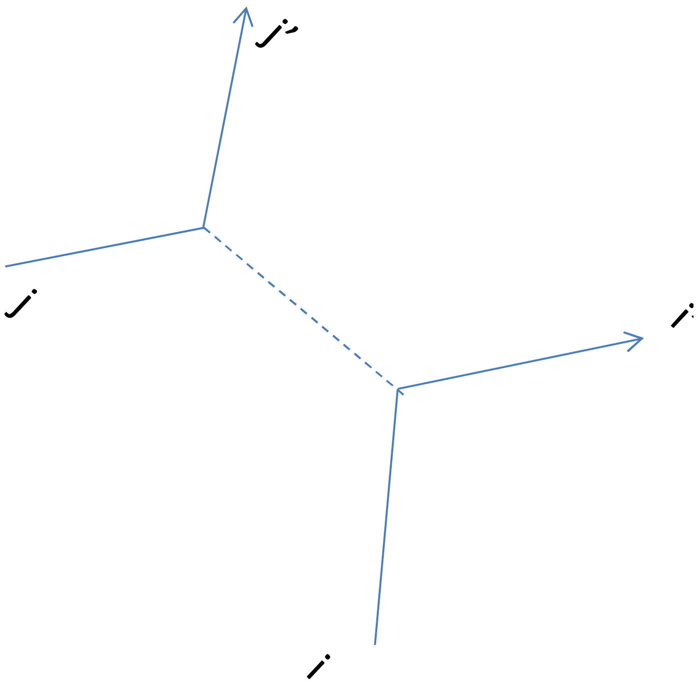
High order correlation in the simulations

		Fermi		Boltzmann		Cascade (60-140 fm/c)	
		$T=0$	$T=5$ MeV	$T=0$	$T=5$ MeV	$T=0$	$T=5$ MeV
Non-relativistic	Num. Int.	118.1 [a]	122.1	115.9 [a]	120.1		
	Cascade	118.2	122.1	115.9	120.1	122.8	127.3
Quasi-relativistic	Num. Int.	115.0	118.8	112.3	116.3		
	Cascade	115.0	118.8	112.3	116.3	119.0	123.2
Relativistic	Num. Int.			111.4	115.4		
	Cascade ($\delta t = \alpha\Delta t$)	114.0	117.8	111.4	115.4	118.1	122.3
	Cascade ($\delta t = \Delta t$)	115.2	119.0	112.7	116.7	118.4	122.7

Results of with Pauli blocking

Pauli-Blocking probability: 1-(1-f1)*(1-f2)

In QMD, fi is calculated in each event



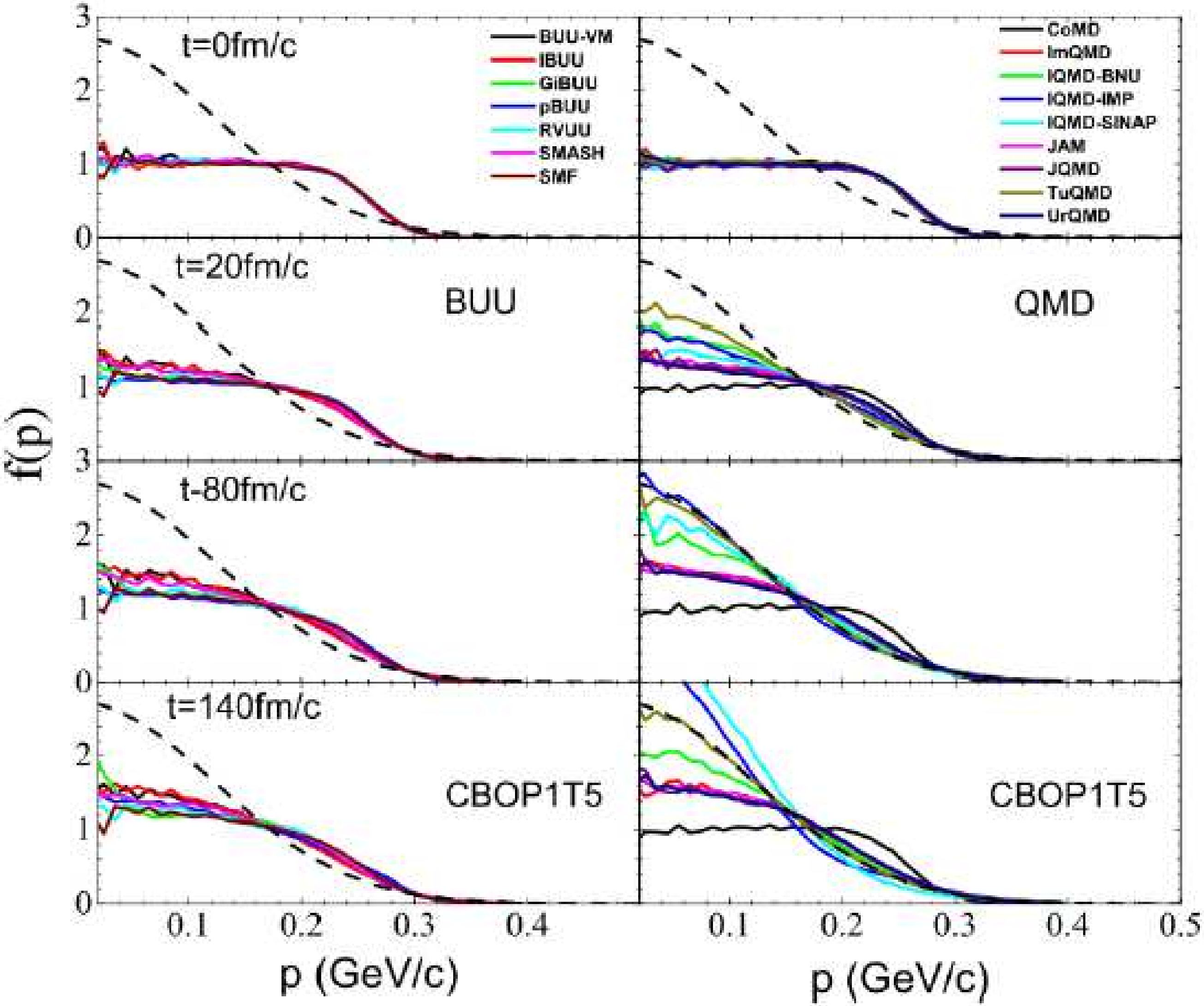
$$
\begin{aligned}
f_i &= f_\tau(\vec{R}_i, \vec{P}_i') \\
&= \frac{1}{2/(2\pi\hbar)^3} \sum_{k\in\tau\,(k\neq i)} \frac{1}{(\pi\hbar)^3} e^{-(\vec{R}_i-\vec{R}_k)^2/2(\Delta x)^2} \\
&\quad \times e^{-2(\Delta x/\hbar)^2(\vec{P}_i'-\vec{P}_k)^2} \\
&= 4 \sum_{k\in\tau\,(k\neq i)} e^{-(\vec{R}_i-\vec{R}_k)^2/2(\Delta x)^2} e^{-2(\Delta x/\hbar)^2(\vec{P}_i'-\vec{P}_k)^2},
\end{aligned} \tag{14}
$$

In BUU, fi is obtained from all test particles

TABLE V: Pauli-blocking treatments used in various codes compared in box calculations.

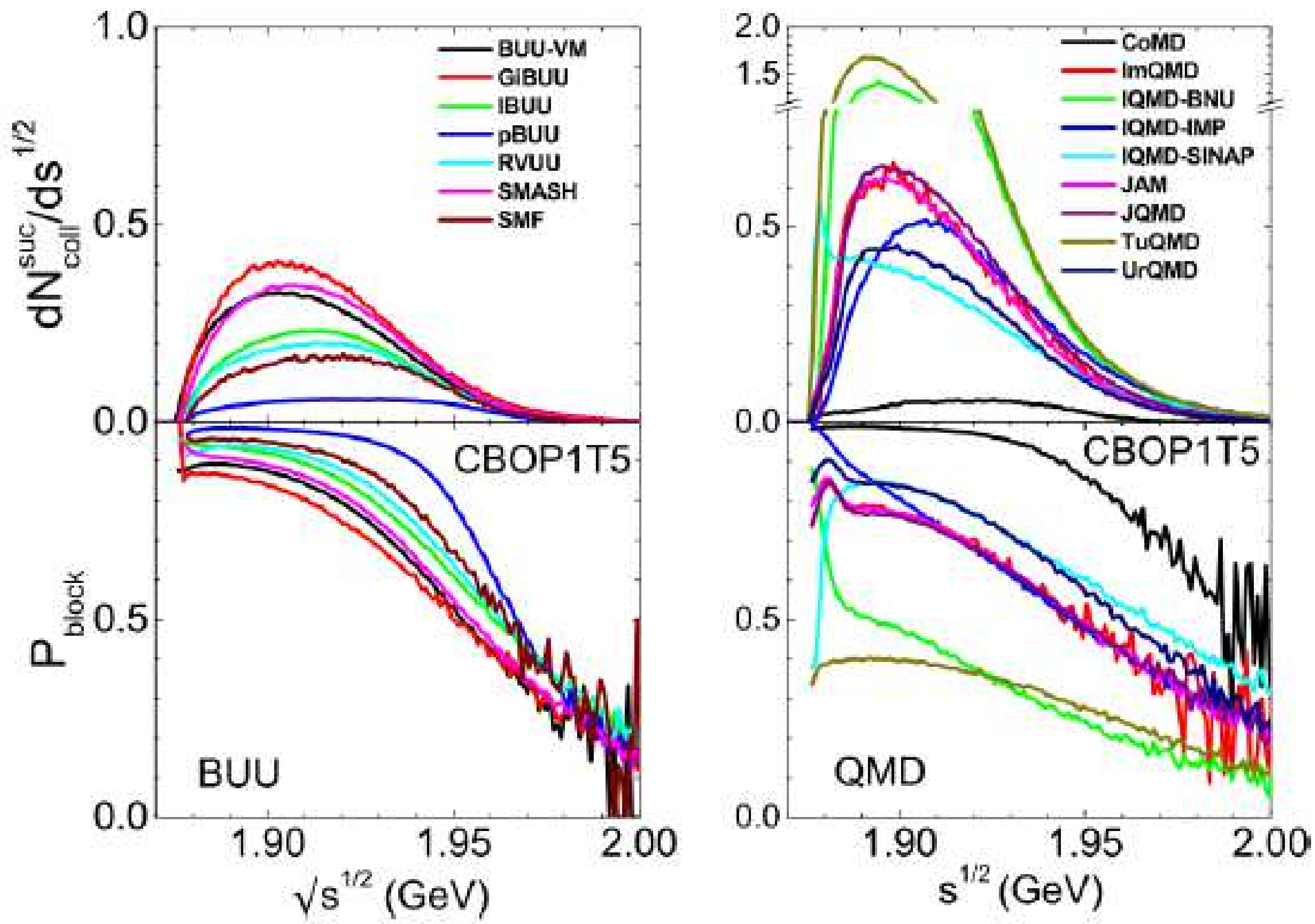
Code name	Occupation probability f_i	Blocking probability[a]	Additional constraints
BUU-VM	f_i in a sphere with $R_x =$ fm, $R_p =$ MeV/c	$1-(1-f_i)(1-f_j)$	no
GiBUU	f_i in phase-space cell with $dx = 1.4$ fm, $dp = 68$ MeV/c	$1-(1-f_i)(1-f_j)$	no
IBUU	f_i in phase-space cell with $dx = 2.0$ fm, $dp = 100$ MeV/c[b]	$1-(1-f_i)(1-f_j)$	no
pBUU	f_i in same and adjacent spatial cells[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[d]	$1-(1-f_i)(1-f_j)$	no
SMASH	f_i in a sphere with $dp = 80$ MeV and $dx = 2.2$ fm[e]	$1-(1-f_i)(1-f_j)$	no
SMF	f_i in sphere with radius 2.53 fm with Gaussian weight in momentum space[f]	$1-(1-f_i)(1-f_j)$	no
CoMD	f_i in h^3 (need comments from Massimo.)	$f_i', f_j' < f_{max} = 1.05 - 1.1$	yes[g]
ImQMD	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ h $(\Delta x)^2 = 2$ fm^2	$1-(1-f_i)(1-f_j)$	no
IQMD-BNU	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ $(\Delta x)^2 = 2$ fm^2	$1-(1-f_i)(1-f_j)$	yes[i]
IQMD-IMP	$f_i = \sum_{k\neq i} V^{ik}_{overlap}/V_0$ with the hard sphere overlap volume $V^{ik}_{overlap}$ determined by $dx = 3.367$ fm, $dp = 89.3$ MeV/c (need comments from Zhao-Qing.)	$1-(1-f_i)(1-f_j)$	no
IQMD-SINAP	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ (Δx =?)	$1-(1-f_i)(1-f_j)$	no
JAM	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ with $(\Delta x)^2 = 2$ fm^2	$1-(1-f_i)(1-f_j)$	no
JQMD	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ $(\Delta x)^2 = 2$ fm^2	$1-(1-f_i)(1-f_j)$	no
TuQMD	$f_i = \sum_{k\neq i} V^{ik}_{overlap}/V_0$ with the hard sphere overlap volume $V^{ik}_{overlap}$ determined by $dx = 3.0$ fm, $dp = 240$ MeV/c[j]	$1-(1-f_i)(1-f_j)$	yes[k]
UrQMD	$f_i = 4\sum_{k\in\tau(k\neq i)} e^{-(R_k-R_i)^2/(2(\Delta x)^2)} e^{-(P_k-P_i')^2\cdot 2(\Delta x)^2/\hbar^2}$ (Δx =?)	$1-(1-f_i)(1-f_j)$	yes[l]

Time evolution of momentum distribution for CBOP1T5



1, evolve toward to Boltzmann distribution

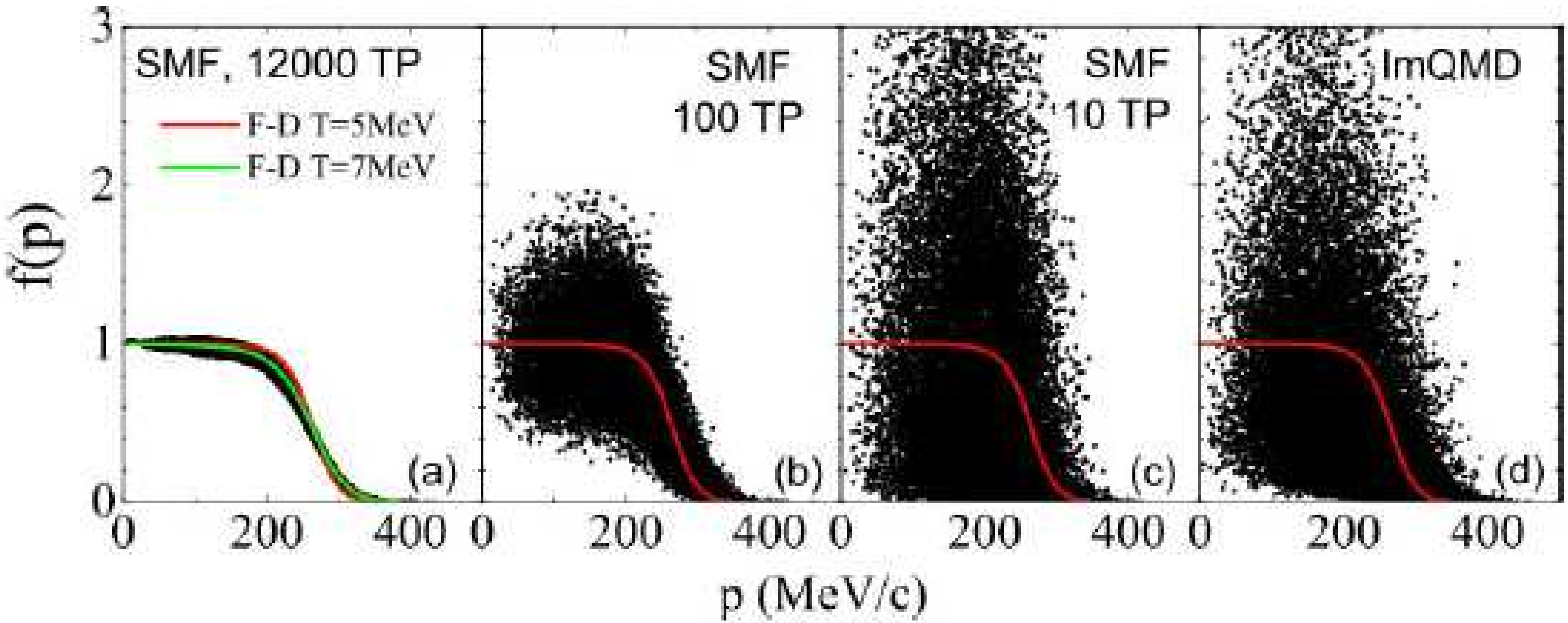
2, BUU code is better, while QMD is worse except for CoMD



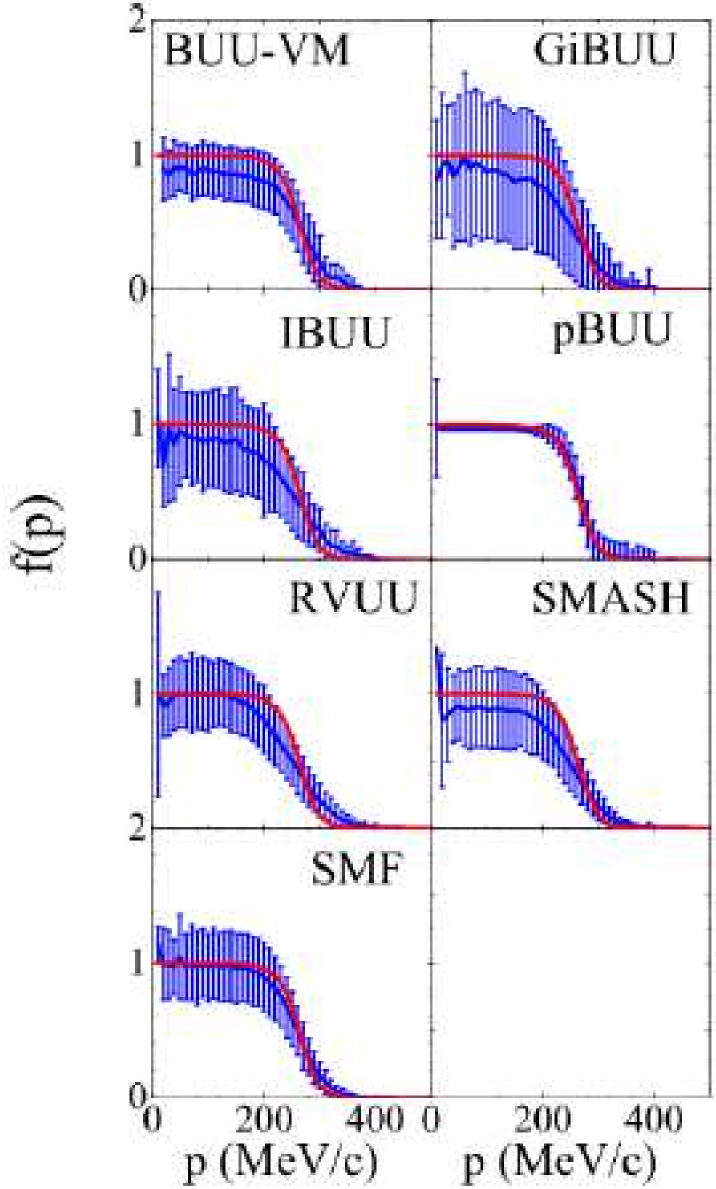
1, The majority of attempted collisions occur at low energy relative to the threshold where the collisions should be suppressed most effectively.

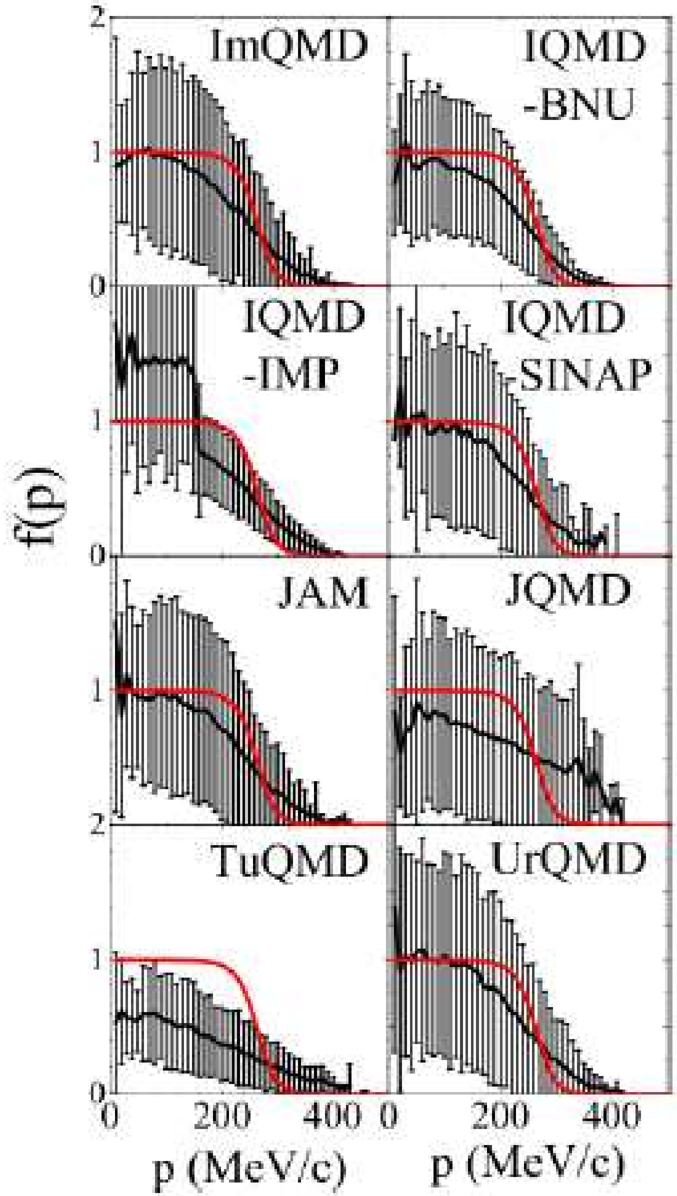
2, By the Fermi energy, the collision rates are seen to converge better between the codes as the blocking becomes less important.

Pauli blocking only for the first time step



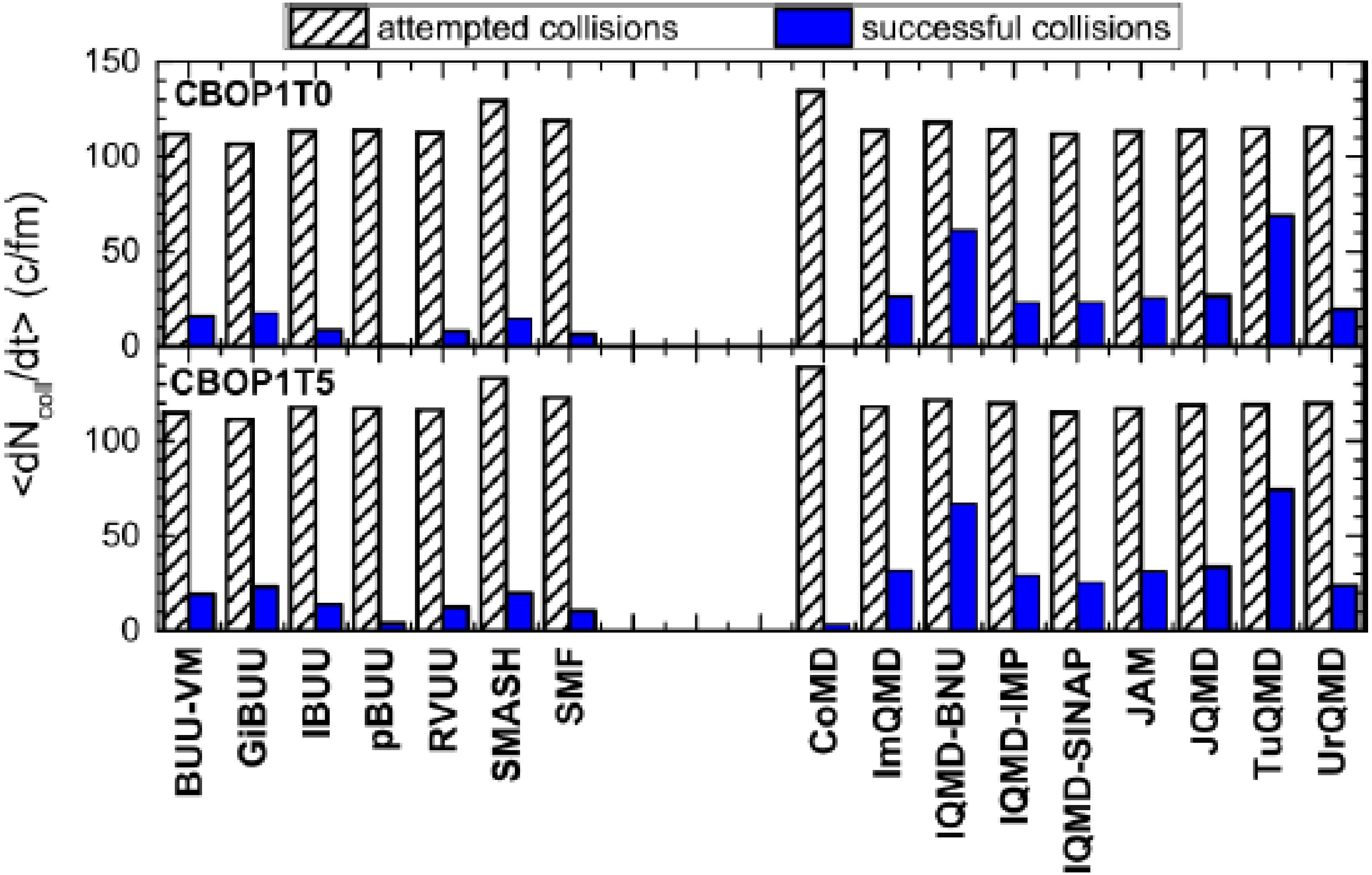
- Fluctuation in occupation probability, and can be reduced by increasing N_tp or width of wf
- a large fluctuation leading to low occupation probabilities, collisions could occur where they should be forbidden.





- BUU codes systematically give a smaller variance compared to QMD codes

Time averaged collision rate for CBOP1



- Successful collision rates for QMD are considerably higher than the BUU
- both QMD and BUU can not reach the theoretical limits

Summary and outlook

1, collision probabilities are well under control, after eliminating repeated collisions between the same pair of particles

2, blocking factor is subject to fluctuations which destroy the fermionic character of a system

3, fluctuation are physical in heavy ion collisions and lead to observable effects. Thus they should not be arbitrarily suppressed. **The question of how to control the fluctuation in transport theories remains an open one.**

- HW2 for BOX simulations, Mean field propagation, fluctuations, are on going

Maria Colonna’s talk

- HW3 for BOX simulations, pion productions, are on going

Akira Ono’s talk

Thanks for your attention!