# HEAVY-ION COLLISIONS IN THE FLUKA MONTE CARLO EVENT GENERATOR: PRESENT AND PERSPECTIVES

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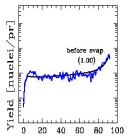
The incorporation of models which simulate heavy-ion collisions into the FLUKA Monte Carlo transport code is in progress [1,2]. While the DPMJET module has been succesfully employed at energies of several GeV/A [3], at lower energies, ranging from a few hundreds of MeV/A up to few GeV/A, preliminary results were obtained using a modified version of the Sorge relativistic RQMD code [8], coupled with specific FLUKA evaporation/fragmentation/fission routines.
Furthermore, a QMD code written from scratch by the authors, is under development. As a starting project, this code is designed to cover the energy range of a few hundreds of MeV/A, planning its extension to relativistic energies as a further step. Particular effort is devoted to the study of the nucleon - nucleon interaction potential, connecting it to the mean single - particle nuclear potential, inferred from experimental data. The effect of various terms is shown, and in particular the role of the so - called surface term in creating the potential dip at the nuclear surface and in preserving a reasonable phase - space occupation around each nucleon is underlined. A connection with the nucleon gaussian width choice is established. A few comments regarding the surface - symmetry correction, recently included in the ImQMD-II model [13], are also made. Specific methods to take into account antisymmetrization effects in QMD models, such as the inclusion of a Pauli potential or the implementation of the phase - space CoMD constraint [19], are critically reviewed, showing their advantages and their shortcomings.

## RQMD

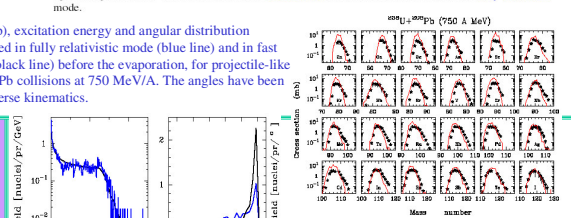
### The RQMD 2.4 - FLUKA interface

The Sorge RQMD 2.4 code [8] is a Monte Carlo code used to simulate heavy-ion collisions at relativistic bombarding energies. The model is based on the principles of the Poincaré invariant Constrained Hamiltonian Dynamics. The constraints allow a reduction of the 8N dimensional phase space to the usual non relativistic 6N dim. phase space (N = number of particles): N of them force the particles to move on energy shell between collisions, while the remaining N fix the relative time among particles and relate the time of all particles to a global evolution parameter. The constraints determine the Dynamics: the Hamiltonian is fully relativistic and is given by their combination.
The code was interfaced to FLUKA [2] adding
* a projectile-like and a target-like residual definition scheme,
* a procedure to calculate the fragment excitation energies at the end of the dynamical stage, which are absent in the original RMQD 2.4 code version. Further,
* the code has been coupled to the FLUKA evaporation/fusion/fragmentation module.

Specific options allow to switch between the fast-cascade mode (INC like mode) and the fully relativistic mode.




Charge yield (up), excitation energy and angular distribution (down), computed in fully relativistic mode (blue line) and in fast cascade mode (black line) before the evaporation, for projectile-like residuals of U+Pb collisions at 750 MeV/A. The angles have been evaluated in inverse kinematics.







Projectile-like fragment cross section (computed in fast cascade mode) after the evaporation, compared to experimental data [9].

## QMD MODEL DEVELOPMENT

### From a nucleon-nucleon effective potential to the total nuclear potential energy

Skyrme II + symmetry + Coulomb + surface + Skyrme III

The matrix elements of the effective interaction hamiltonian operator in coordinate space, which describe the effect on a particle of charge $C_i$ located in $\mathbf{r}$ due to another particle $j$ located in $\mathbf{r}'$ (or due to two other particles in $\mathbf{r}'$ and $\mathbf{r}''$), are assumed to be:

$$H^{(2)}_{\mathrm{Int_+S.P.}}(C_i\mathbf{r},C_j,\mathbf{r}') = \frac{\alpha}{\rho_0}\delta(\mathbf{r}-\mathbf{r}') + \frac{C_{is}}{\rho_0}\delta(\mathbf{r}-\mathbf{r}')[2\delta(C_{is}C_j)-1] + \frac{e^2}{4\pi\epsilon_0|\mathbf{r}-\mathbf{r}'|} +$$
$$- \frac{g_{\mathrm{surf}}}{4}\left[\left(\overrightarrow{\nabla}-\overrightarrow{\nabla}'\right)^2\delta(\mathbf{r}-\mathbf{r}')+\delta(\mathbf{r}-\mathbf{r}')\left(\overrightarrow{\nabla}-\overrightarrow{\nabla}'\right)^2+2\left(\overrightarrow{\nabla}-\overrightarrow{\nabla}'\right)\delta(\mathbf{r}-\mathbf{r}')\left(\overrightarrow{\nabla}-\overrightarrow{\nabla}'\right)\right],$$
$$H^{(3)}_{\mathrm{Int_+S.P.}}(\mathbf{r},\mathbf{r}',\mathbf{r}'') = \frac{2\beta}{\rho_0^2}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}'').$$

The single-particle potential can be calculated by:

$$V_{\mathrm{S.P.}}(\mathbf{r}) = V^{(2)}_{\mathrm{S.P.}}(\mathbf{r}) + V^{(3)}_{\mathrm{S.P.}}(\mathbf{r}) =$$
$$= \sum_j \int d^3r'\phi_j^*(\mathbf{r}')H^{(2)}_{\mathrm{Int_+S.P.}}(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r}') +$$
$$+ \frac{1}{2}\sum_j\sum_{k\neq j}\int d^3r'd^3r''\phi_j^*(\mathbf{r}')\phi_k^*(\mathbf{r}'')H^{(3)}_{\mathrm{Int_+S.P.}}(\mathbf{r},\mathbf{r}',\mathbf{r}'')\phi_j(\mathbf{r}')\phi_k(\mathbf{r}'')\,,$$

and the total potential energy is given by:

$$V = V^{(2)}+V^{(3)} =$$
$$= \frac{1}{2}\sum_i\sum_{j\neq i}\int d^3r\,d^3r'\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')H^{(2)}_{\mathrm{Int_+S.P.}}(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r})\phi_j(\mathbf{r}') +$$
$$+ \frac{1}{6}\sum_i\sum_{j\neq i}\sum_{k\neq i,j}\int d^3r\,d^3r'\,d^3r''\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')\phi_k^*(\mathbf{r}'')H^{(3)}_{\mathrm{Int_+S.P.}}(\mathbf{r},\mathbf{r}',\mathbf{r}'')\phi_i(\mathbf{r})\phi_j(\mathbf{r}')\phi_k(\mathbf{r}'')\,.$$

### The potential parameters

* $\alpha$, $\beta$, ($\gamma = 2$) were fixed to reproduce the properties of symmetric infinite nuclear matter: binding energy, saturation, (compressibility $\sim 380$ MeV $\leftarrow$ hard EOS).
* $C_{is}$ was fixed to produce a symmetry energy contribution in agreement with the semi-empirical mass formula.
* $g_{\mathrm{surf}}$ can not be constrained on the basis of nuclear matter properties ($\nabla_{\mathbf{r}}\rho = 0$). It was then fixed to reproduce the empirical single-particle central potential wells (as predicted by Koura et al. [10]) as closest as possible. This leads to:

$$g_{\mathrm{surf}} = -\frac{\alpha\,\sigma_r^4}{\rho_0\,(r_0^2+3\,\sigma_r^2)}\,,$$

where $r_0^2$ has the same order of magnitude of typical nucleon-nucleon square distances averaged over the whole nucleus. Note the surface parameter value dependence on the choice of the nucleon gaussian width $\sigma_r$.

| $\alpha$ | $\beta$ | $\rho_0$ | $C_{is}$ | $g_{\mathrm{surf}}$ | $r_0^2$ |
|---|---|---|---|---|---|
| $-125.39$ MeV | 71.03 MeV | 0.17 fm$^{-3}$ | 46 MeV | $\sim \frac{-\alpha\sigma_r^2}{\rho_0(r_0^2+3\sigma_r^2)}$ | $\frac{1}{A(A-1)}\sum_i\sum_{j\neq i}(\mathbf{R}_i-\mathbf{R}_j)^2$ |

### The surface interaction versus the Yukawa interaction

* The Yukawa potential is always attractive, both at long distances and at the shorter ones.
* The surface term is splitted in an attractive component, acting especially at the nuclear surface, and in a repulsive core, that helps taking into account the repulsive nucleon-nucleon short range correlations.

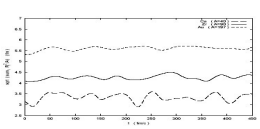
⇒ While the surface term is effective in preserving nuclear stability [11], the introduction of a Yukawa term is better accomplished together with the inclusion of a Pauli potential in the nuclear Hamiltonian [12], to avoid the nucleons coming too close in phase-space during time evolution and the occurrence of spurious emissions.

### QMD potential has been improved by The surface-symmetry correction term

$$V_{\mathrm{sea-sky}} = \frac{C_{is}\beta_{ss}}{\rho_0}\frac{1}{2L(4\pi\sigma_r^2)^{3/2}}\sum_i\sum_{j\neq i}(2C_i-1)(2C_j-1)\left[3-\frac{(\mathbf{R}_i-\mathbf{R}_j)^2}{2\sigma_r^2}\right]e^{-\frac{(\mathbf{R}_{ij}-\mathbf{R}_{ij}')^2}{4\sigma_r^2}}.$$

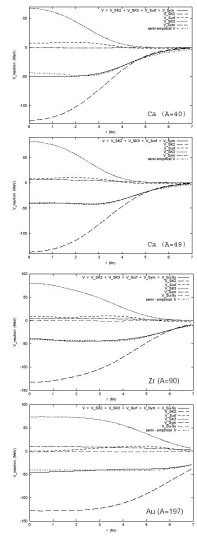
It corrects the surface term [13],
* smoothing its effect for $nn$ and $pp$ pairs,
* increasing its effect for $np$ pairs.

⇒ Improved nuclear stability: the QMD ground states remain stable for $\sim 400-500$ fm/c.



R.m.s. radius time evolution for selected Ca, Zr and Au configurations.

### Single – particle potential for neutrons in Ca, Zr, Au nuclei




### Nucleons as fermions

*In QMD models the total nuclear wave function is assumed to be the product of single nucleon wave functions.
*The proper way to take into account the Pauli Exclusion Principle consists in antisymmetrizing the nuclear wave function, as done in some extensions of QMD models (like FMD [14] and AMD [15]). However, this becomes computationally prohibitive with increasing nuclear mass.
*Historically, before the introduction of these models, both in the context of Classical Molecular Dynamics and in the context of its Quantum versions, some groups (see, e.g., [16,17]) proposed to include a Pauli potential to simulate in some approximated way the Pauli Principle.

$$V_{ij}^{\mathrm{Pauli}} = V(\vec{R}_{ij}, \vec{P}_{ij}, S_{ij})$$

Its expression implies that the closer the nucleons $ij$ are in the coordinate space, the more they will be forced apart in the momentum space. In general, it involves many parameters that can be fixed by imposing that the energies of a free Fermi gas (simulated by a Metropolis algorithm [12] or by damping equations of motion [18]) match their exact theoretical values for a wide range of temperatures and densities. The main advantage of the Pauli potential is that it leads to well-defined ground states.

BUT

# $\vec{R}_i$ and $\vec{P}_i$ are NOT the mean position and momentum of a given particle, they are NOT canonically conjugated variables. ⇒ The equation of motion should be rederived [14].

# Concerning the experimental data simulation, it has been claimed that including a Pauli potential gives rise to spurious repulsion during the collisions (see, e.g., [19]).

# From a technical point of view, including it in the initialisation stage is not immediate, at least if one wants to match the experimental constraints on the ground state binding-energy values.

### The CoMD constraint

The authors of ref. [19] proposed a constraint to prevent the nucleons coming too close to each other in phase-space:

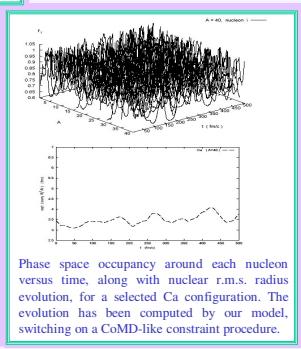
$$< f_i > \equiv \sum_j \delta_{\tau_i\tau_j}\delta_{s_is_j}\int_{j3}f_j(\mathbf{r},\mathbf{p})\,d\mathbf{r}d\mathbf{p} \leq 1\,, \quad \text{for } i=1,...,A\,,$$

where $\tau_{i(j)}$ and $s_{i(j)}$ represent the isospin and spin quantum numbers, respectively. The integration is performed on a phase-space hypercube of volume $h^3$ centered on the centroid coordinates $(\mathbf{R}_i, \mathbf{P}_i)$, with linear size $\sqrt{4\pi\sigma_r^2}$ in coordinate space and $\sqrt{\pi h^2/\sigma_r^2}$ in momentum space.

In particular, when a nucleon or more violate the condition above, the solution consists of randomly changing their momenta and the momenta of the closest particles, imposing the total kinetic energy and the total nuclear momentum conservation.
⇒ This implementation does not affect the nucleon positions.
⇒ It simulates many-body scattering effects.

BUT

# Differently from the Pauli potential, abrupt and random changes of the $\mathbf{P}_i$ momentum values are introduced.
# The evolution of each nucleus is not uniquely determined by the initial nucleon centroid coordinates, since it also depends on many random numbers, which should be stored as well, to use the configuration again in the simulation of nucleus-nucleus collisions....

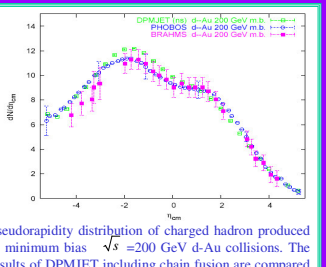


Phase space occupancy around each nucleon versus time, along with nuclear r.m.s. radius evolution, for a selected Ca configuration. The evolution has been computed by our model, switching on a CoMD-like constraint procedure.

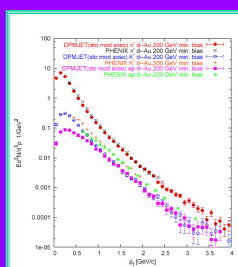
## DPMJET

### The DPMJET-III code system

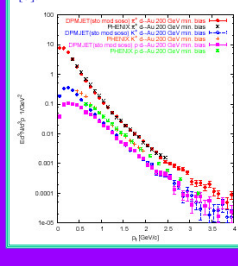
The DPMJET-III Monte Carlo code [3] simulates the interactions involving hadrons, nuclei and photons from a few GeV/A up to cosmic ray energies. The collisions involving nuclei are treated according to the Glauber-Gribov theory, and the elementary collisions are implemented on the basis of perturbative QCD results and the Dual Parton Model [4], a phenomenological model suitable to describe soft multiparticle production. At present, RHIC data can be used to tune some properties of the soft part of the model, which cannot be derived using perturbative QCD. In particular, the available exp. data on Au-Au and d-Au collisions at $\sqrt{s} = 200$ GeV [5] have shown the importance of adding percolation and chain fusion schemes, which have been implemented into the model. Further, a new transverse momentum distribution, on which is based the fragmentation of the soft chains, has been introduced (while in the previous versions of the model the transverse momentum distributions adopted for the soft chains had a gaussian form, as those for the hard chains). Other recent improvements are described in ref. [6].




Pseudorapidity distribution of charged hadron produced in minimum bias $\sqrt{s}$ =200 GeV d-Au collisions. The results of DPMJET including chain fusion are compared to experimental data from the BRAHMS-Collaboration and the PHOBOS-Collaboration [5].




Transverse momentum distribution of negatively (up) and positively (down) charged hadrons in minimum bias $\sqrt{s}$ =200 GeV d-Au collisions. Compared are the data from the PHENIX collaboration to the results of the latest version of DPMJET-III [7].

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