New native QMD code in Geant4

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Quantum Molecular Dynamics

- QMD (Quantum Molecular Dynamics) is quantum extension of classical molecular-dynamics model.
- Each nucleon is seen as a Gaussian wave packet
- Propagation with scattering term which take into account Pauli principals
- QMD model is widely used to analyze various aspects of heavy ion reactions. Especially for many-body processes in particular the formation of complex fragments which hard to treat with Vlasov-Uehling-Uhlenbeck (VUU) and Boltzmann-Uehling-Uhlenbeck (BUU) equations

Derivation of the transport equation of QMD

- Wave function of each nucleon in the system

$$\phi_i(x;q_i,p_i,t)=\left(\frac{2}{L\pi}\right)^{3/4}\exp\left\{-\frac{2}{L}(x-q_i(t))^2+\frac{i}{\hbar}p_i(t)x\right\}$$

- Total n-body wave function

$$\Phi=\prod_i \phi_i(x;q_i,p_i,t)$$

- Hamiltonian

$$H=\sum_i T_i+\sum_{ij}V_{ij}$$

- Equations of motion for i-th particles

$$\dot{p}_i=-\frac{\partial\langle H\rangle}{\partial q_i}\quad and\quad \dot{q}_i=\frac{\partial\langle H\rangle}{\partial p_i}$$

Binary Light Ion Cascade

This is an Ion extension of Binary Cascade

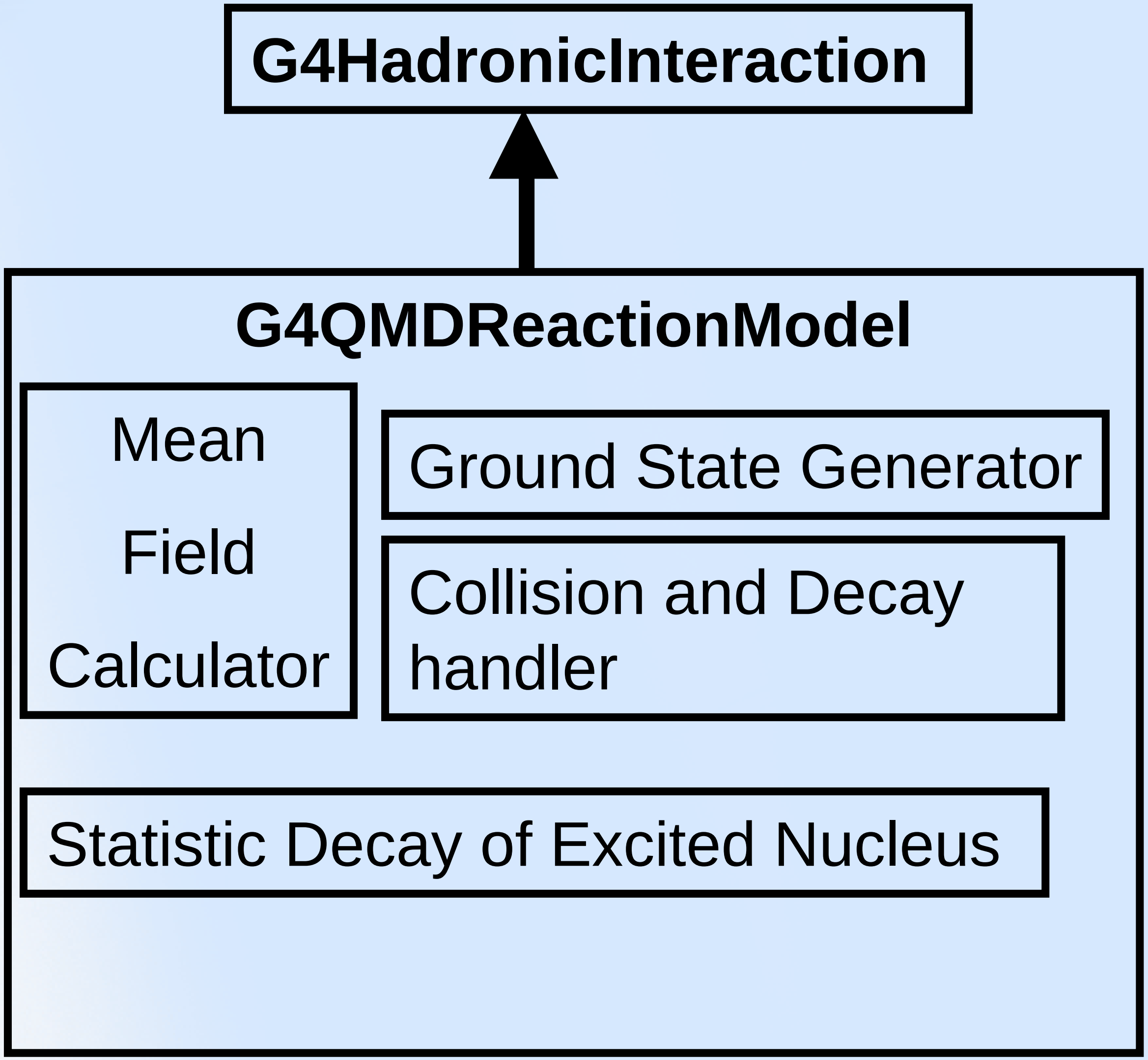
- In Binary Cascade
  - Participant nucleons are also represented by wave function and numerically calculated time development of Hamiltonian
  - The scattering term considers only binary collision and decay
- However, Binary Cascade
  - Neglects participant-participant scattering
  - Uses simple time independent optical potential
  - Does not provide ground state nucleus which can be used in molecular dynamics
- Recommended for use when either projectile or target is C12 or lighter (other particle can be heavier)

G4QMD

The solution for overcoming limitation of Binary Light Ion Cascade, and enable to simulate real HZE reactions

- G4QMD create ground state nucleus based on JQMD, which can be used in MD
- Potential field and field parameters of G4QMD is also based on JQMD with Lorentz scalar modifications
  - "Development of Jaeri QMD Code" Niita et al, JAERI-Data/Code 99-042
- Self generating potential field is used in G4QMD
- G4QMD uses scatter and decay library of Geant4

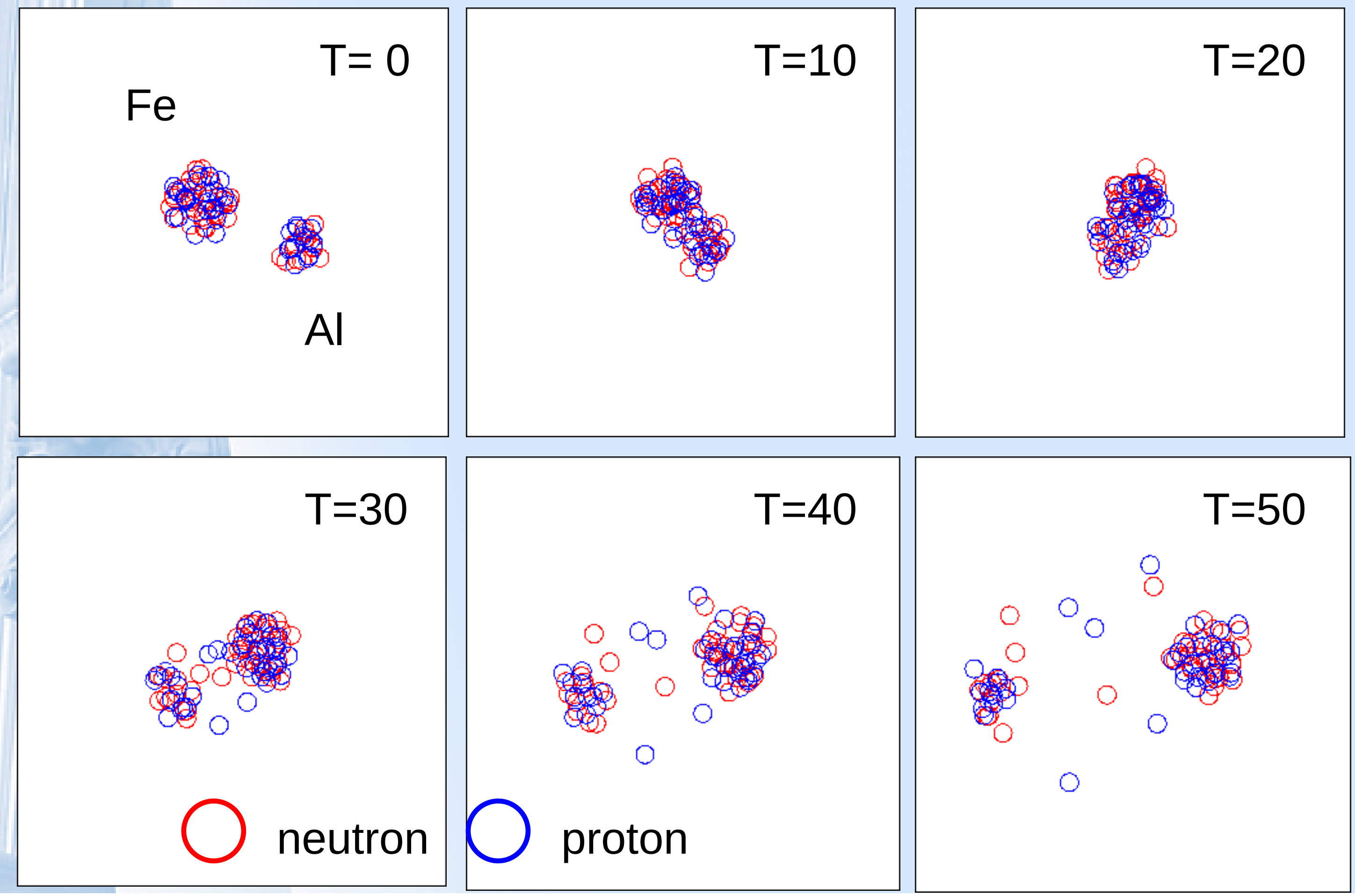
  Following resonances are taken into account
  - Δ_{1232}, Δ_{1600}, Δ_{1620}, Δ_{1700}, Δ_{1900}, Δ_{1905}, Δ_{1910}, Δ_{1920}, Δ_{1930}, and Δ_{1950}
  - N_{1400}, N_{1520}, N_{1535}, N_{1650}, N_{1675}, N_{1680}, N_{1700}, N_{1710} , N_{1720}, N_{1900}, N_{1990}, N_{2090}, N_{2190}, N_{2220} and N_{2250}
- G4QMD includes Participant-Participant Scattering
- After the QMD reaction calculation G4QMD connects to Evaporation Models of Geant4


G4HadronicInteraction
G4QMDReactionModel
Mean Field Calculator
Ground State Generator
Collision and Decay handler
Statistic Decay of Excited Nucleus

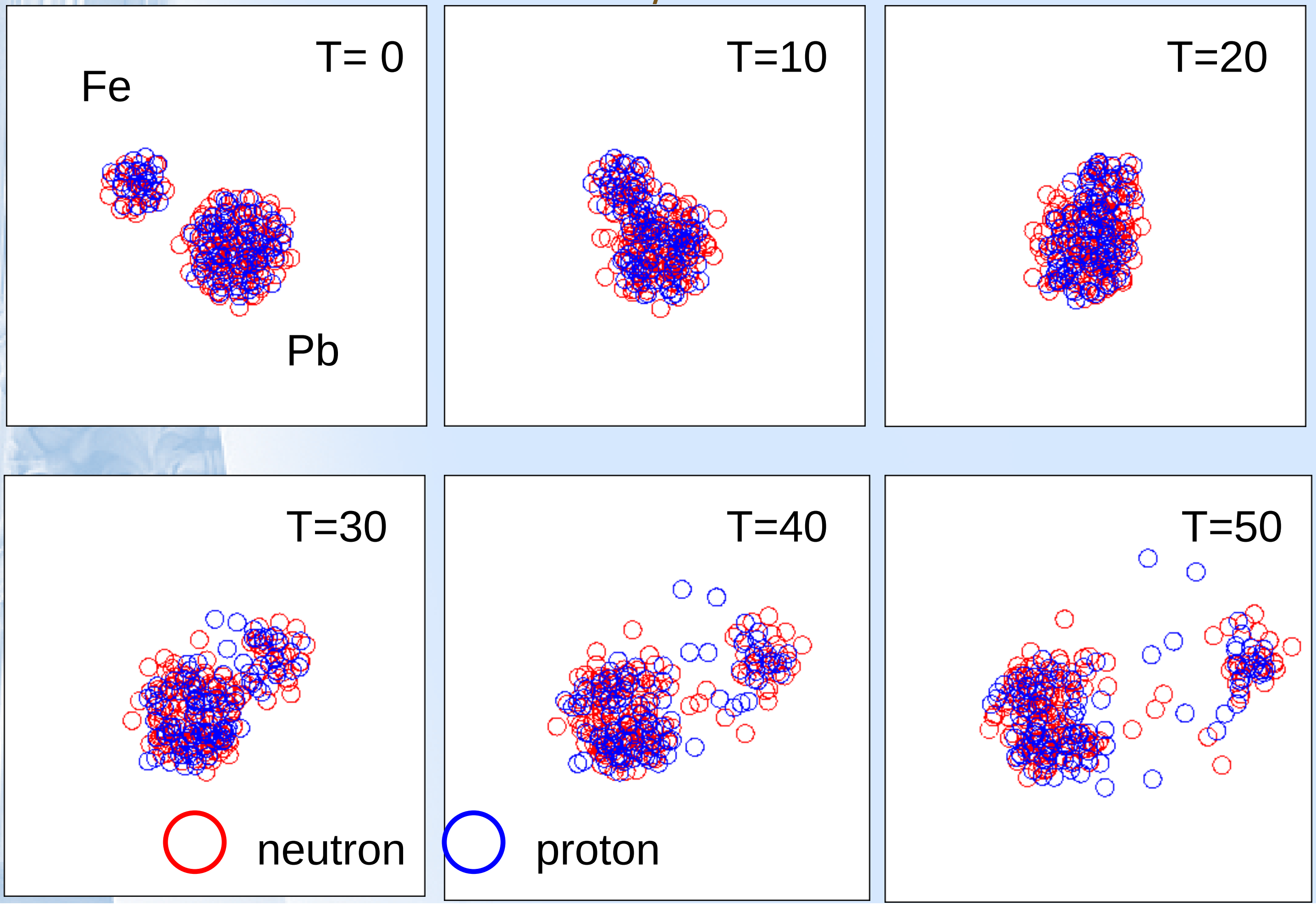
Other features

- Automatic Extension of time steps for relatively slow projectiles.
- Acceleration by Coulomb potential of final state particles is taken into account.
- Above features are incorporated by fruitful discussions with Vanderbilt Univ. group

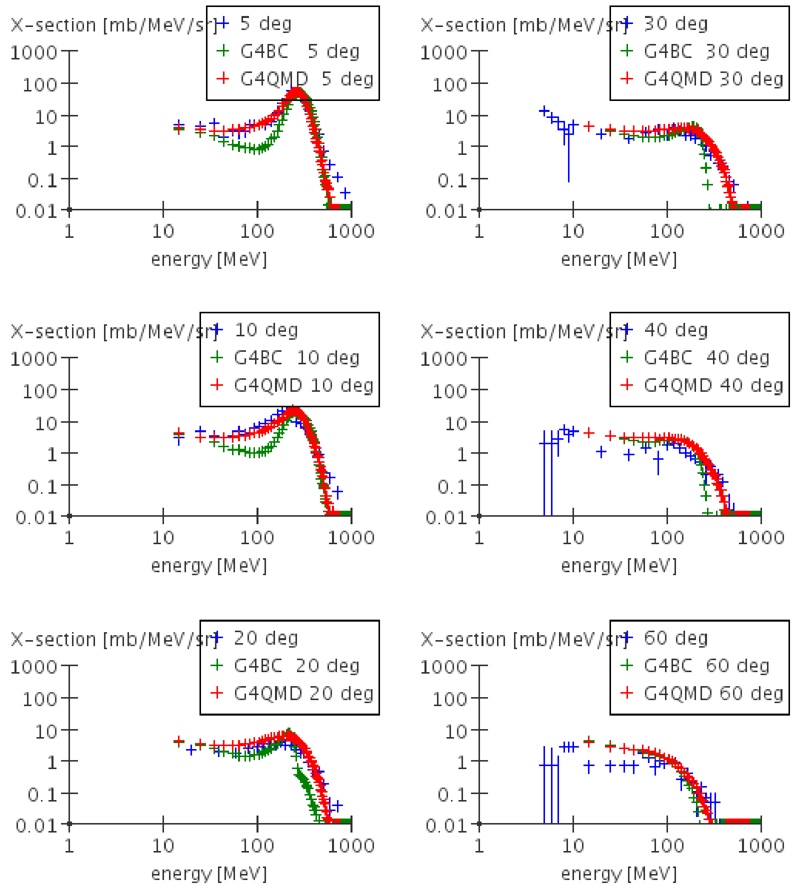
QMD Calculation
Fe 290MeV/n on Al



QMD Calculation
Fe 290MeV/n on Pb

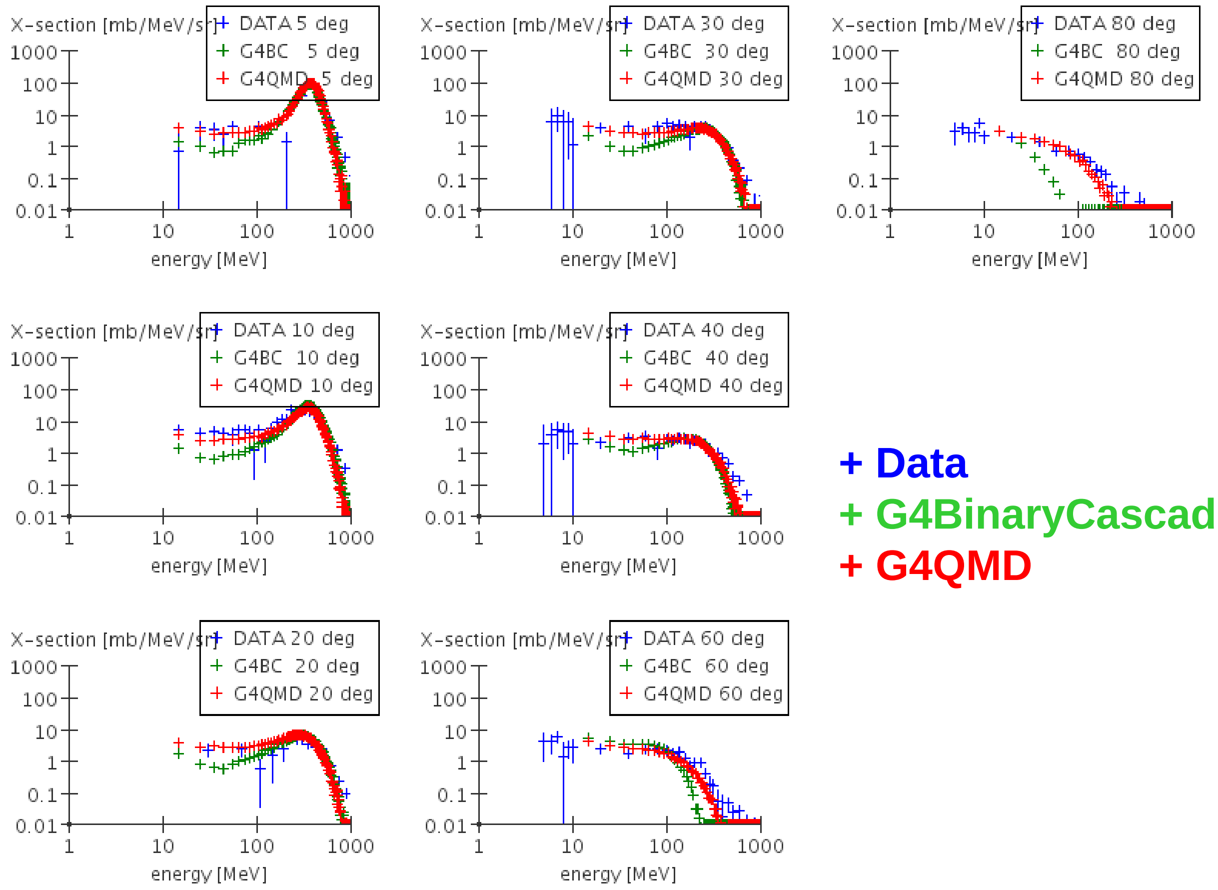


C12 290MeV/n on Carbon Secondary neutron spectra



+ Data
+ G4BinaryCascade
+ G4QMD

Ne20 400MeV/n on Carbon
Secondary neutron spectra

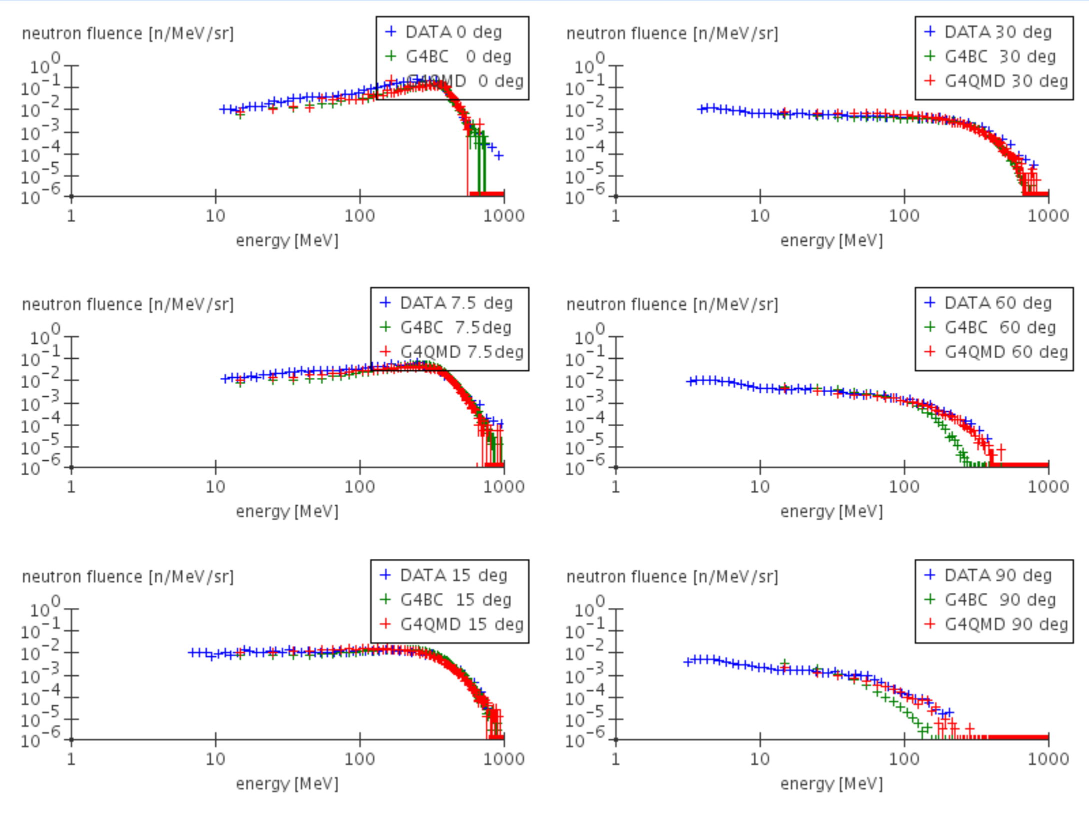


+ Data

+ G4BinaryCascade

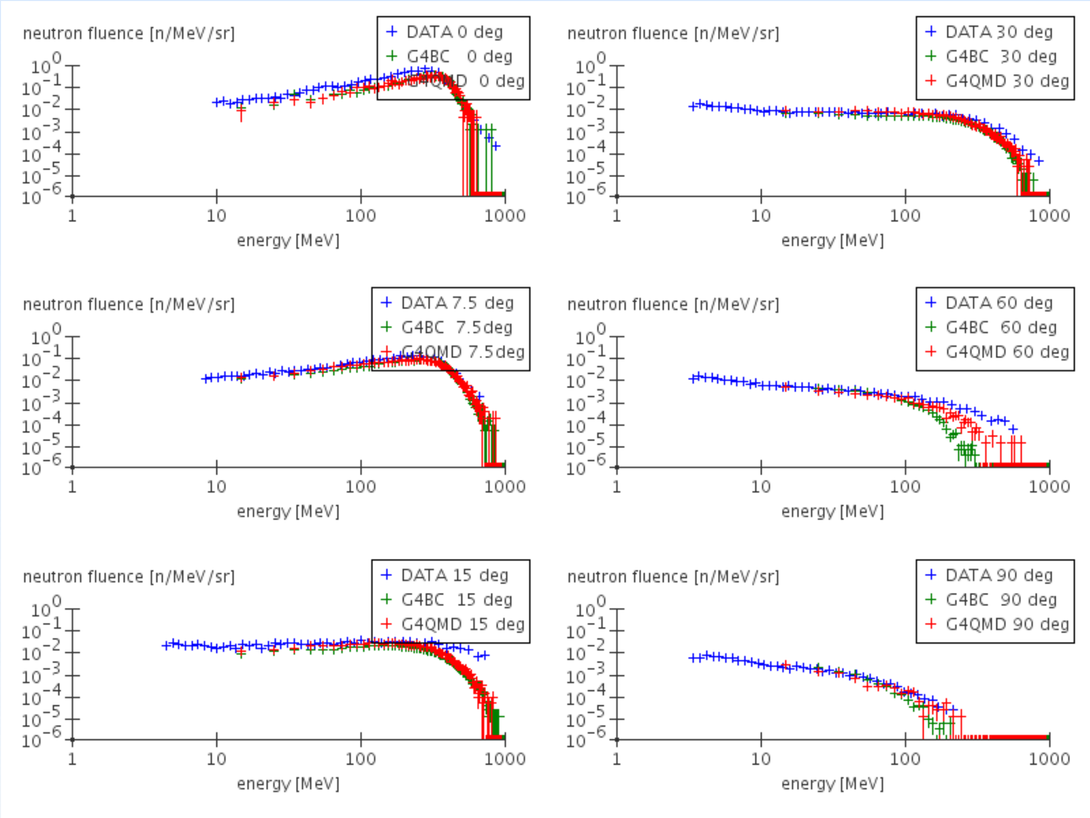
+ G4QMD

Fe56 400MeV/n on Thick Aluminum Neutron Yield



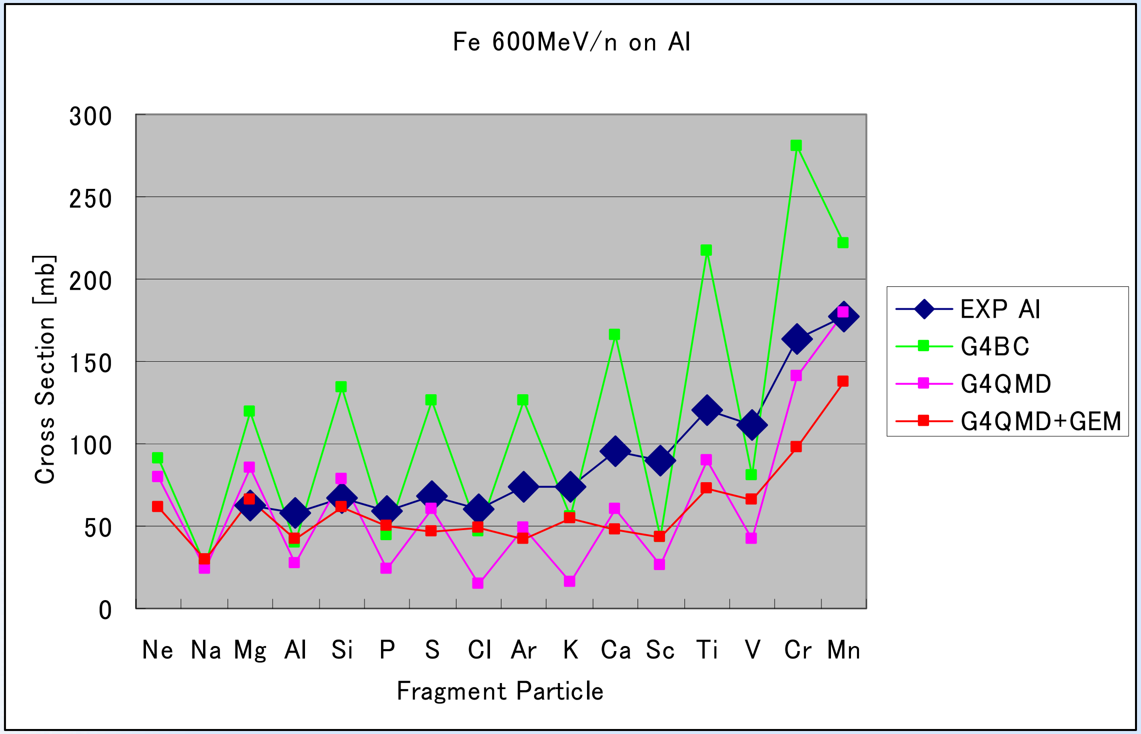
+ Data, + G4BinaryCascade, + G4QMD

Xe132 400MeV/n on Thick Aluminum Neutron Yield



+ Data, + G4BinaryCascade, + G4QMD

Fragment Particle Production Fe56 600MeV/n on Al



Lorentz covariant dynamics approach

- Should be take care in relativistic energies
- JQMD is not fully Lorentz covariant.
- Sorge et al. formulated Relativistic QMD in fully covariant way based on Poincaré-invariant constrained Hamiltonian dynamics.

Lorentz covariant dynamics approach (2)

- 8N-dimensional phase space

  6N configuration- and momentum-space + 2N Eigen time and energy
- Physical events are described as world lines in the 6n-dimensional phase space
- 8N-dimensional phase space should be constrained 2n-1 degree of freedom and have 6N+1(grobal time τ) degree of freedom

- N mass-shell constraints

$$H_i = p_i^2 - m_i^2 - V_i = 0$$

- And N-1 constraints which connect the relative times of the particles

$$\chi_i = \sum_{j \neq i} g_{ij} p_{ij} q_{ij} = 0$$

$$q_{ij} = q_i - q_j, \quad p_{ij} = p_i + p_j, \quad g_{ij} = \exp\left(q_{ij}^2 / L \right) q_{ij}^{-2}$$

Lorentz covariant dynamics approach (3)

- Hamiltonian

$$H = \sum_{i=1}^{N} \lambda_i H_i + \sum_{i=1}^{N-1} \delta\mu_i \chi_i$$

- Equations of motion

$$\frac{dq_j}{d\tau} = \frac{\partial H}{\partial p_j} = 2\lambda_j p_j - \sum_{i=1}^{N} \lambda_i \frac{\partial V_i}{\partial p_j}$$

$$\frac{dp_j}{d\tau} = -\frac{\partial H}{\partial q_j} = \sum_{i=1}^{N} \lambda_i \frac{\partial V_i}{\partial q_j}$$

with the coefficients λ_i

Lorentz covariant dynamics approach (4)

- And λ_i is

$$\lambda_j \approx -\frac{\partial \chi_N}{\partial \tau} S_{Ni}$$

$$\left(S^{-1}\right)_{ij} \equiv \left\{H_i, \chi_j\right\}_{\text{Poisson bracket}}$$

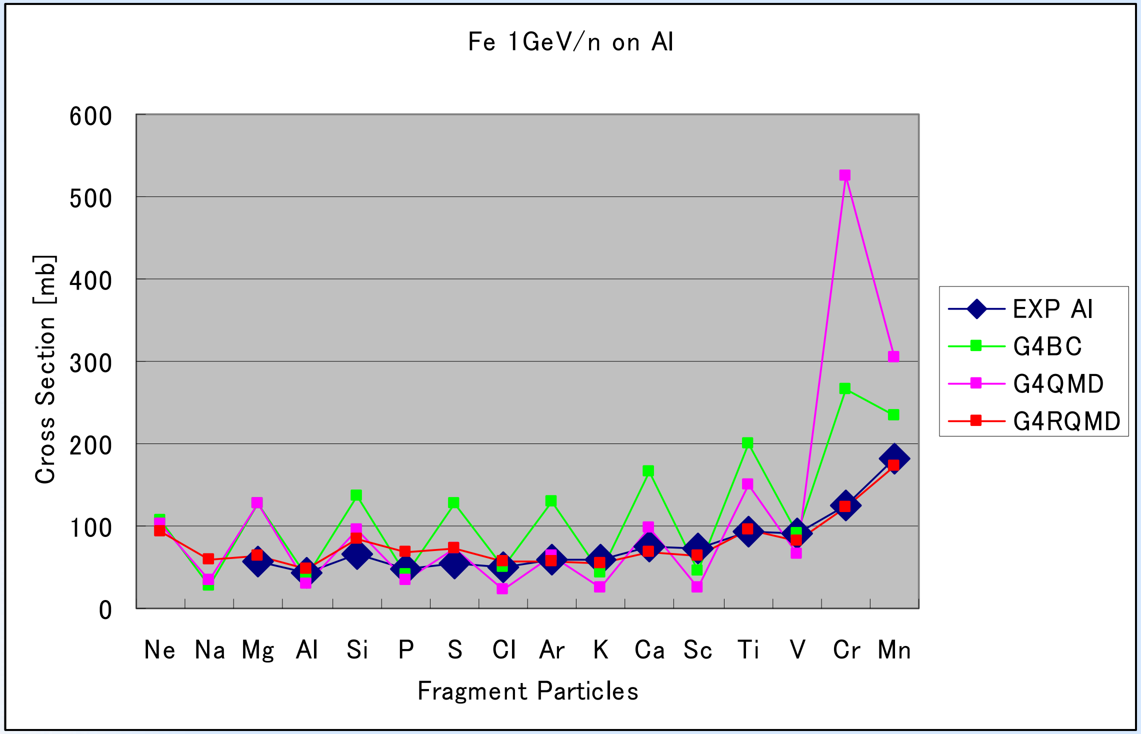
- In order to solve the equations of motion one needs to calculate the coefficients λ_i. For their calculation the matrix S^{-1} must be inverted.

Reference

Poincaré invariant Hamiltonian dynamics: Modelling multi-hadronic interactions in a phase space approach, H. Sorge, H. Stocker and W. Greiner *Ann. Phys*. **192**, 266 1989

Microscopic Models for Ultrarelativistic Heavy Ion Collisions S. A. Bass et al., *Prog. Part. Nucl. Phys*. **41**, 225 1998

Validation of G4RQMD
Fe 1GeV/n on Al



Validation of G4RQMD
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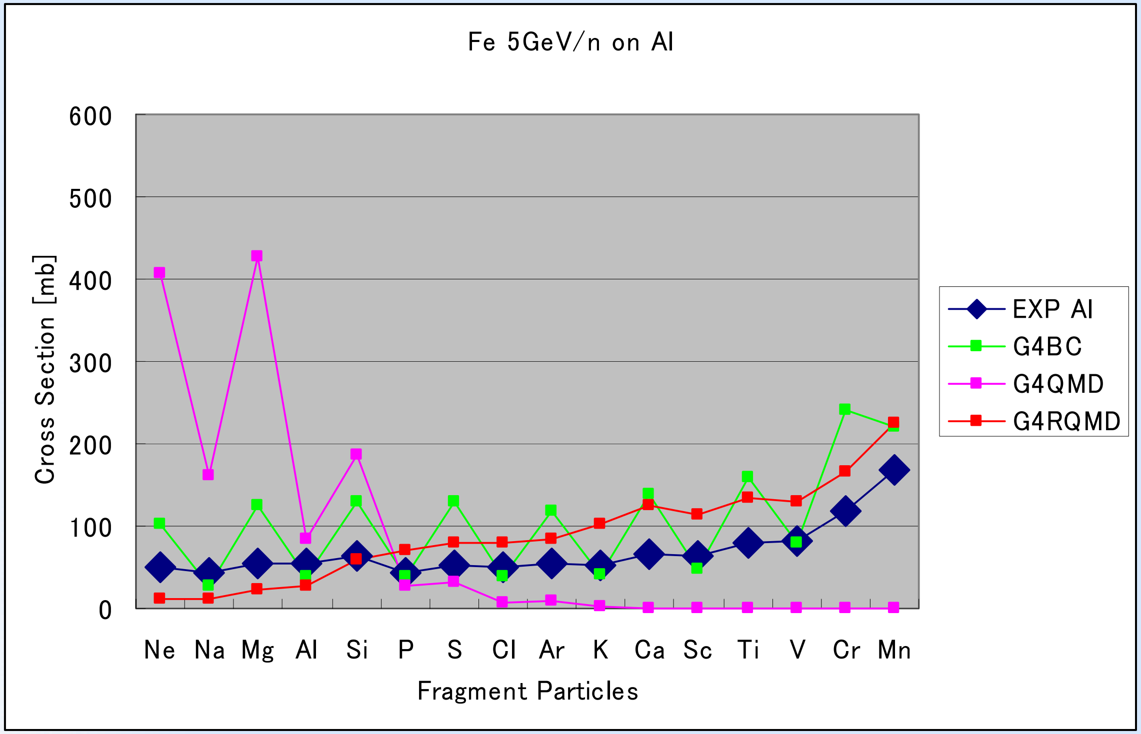

Summary

- We are developing G4QMD which handle nucleus-nucleus interaction up to ~5 GeV/n
- Validation shows much improved results than Binary (Light Ion) Cascade
- The first (alpha) release was done in Geant4 v9.1
- We are also developing G4RQMD which has Lorentz covariant dynamics.
- First validation of G4RQMD shows quite promising results in relativistic energy collisions
- However there still remain many points of improvements and further developments.