New native QMD code in Geant4

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Nucleus collision models in Geant4 until QMD

- Binary Light Ion Cascade Model
  - An Ion extension of Binary Cascade
  - Recommended for use when either projectile or target is C12 or lighter
  - Up to ~10GeV/n
  - More information will be available in the next slide.
- Wilson Abrasion Ablation Model
  - A simplified macroscopic model for nuclear-nuclear interactions based largely on geometric arguments
  - Less detailed model than Binary Cascade or QMD
  - Energy distributions of secondary nucleons are not well described.
  - From 70 MeV/n up to a few tens GeV/n
- Interfacing to other (Fortran) codes outside of Geant4.
  - JQMD, JAM and PHITS (up to 100 GeV/n)
  - DPMJET2 (up to 100 PeV/n)

Binary Light Ion Cascade

- This is an Ion extension of Binary Cascade
- In Binary Cascade
  - Create 3D nucleus model with Pauli principal and Fermi momentum
  - 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)
- The solution for overcoming above limitations of Binary Light Ion Cascade, and enable to simulate real High Z and Energy (HZE) reactions is development of a new native QMD code in Geant4

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 takes into account Pauli principal
- 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 is hard to treat with Vlasov-Uehling-Uhlenbeck (VUU) and Boltzmann-Uehling-Uhlenbeck (BUU) equations

G4QMD(1)

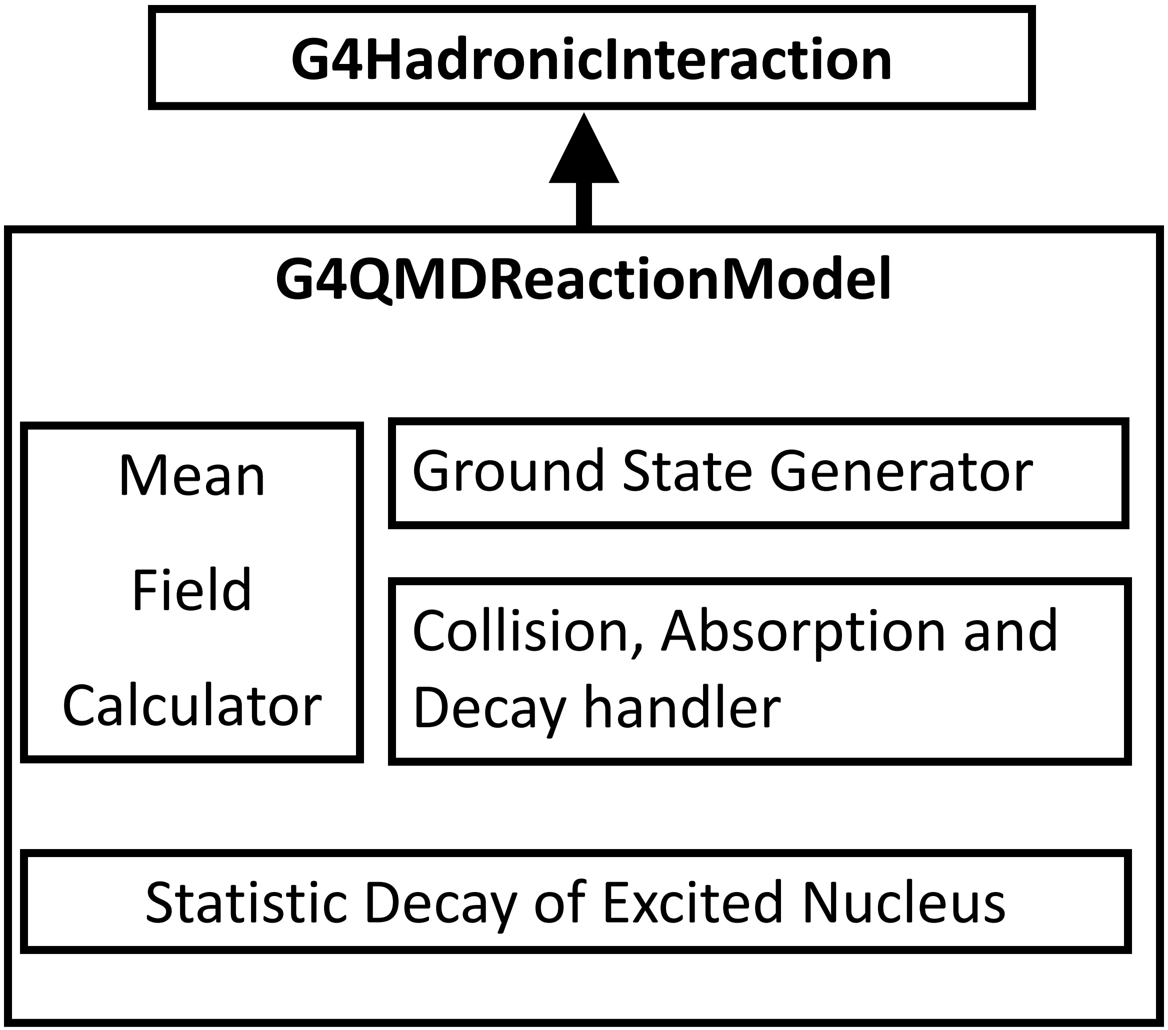
- The solution for overcoming limitation of Binary Light Ion Cascade, and enabling the simulation of real HZE reactions

- 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 scattering and decay library of Geant4
  - Following 25 resonances are taken into account
  - Δ from 1232 up to 1950
  - N from 1400 up to 2250
- G4QMD includes Participant-Participant Scattering
- All major limitations of Binary cascade for Nucleus-Nucleus calculations are cleared in G4QMD

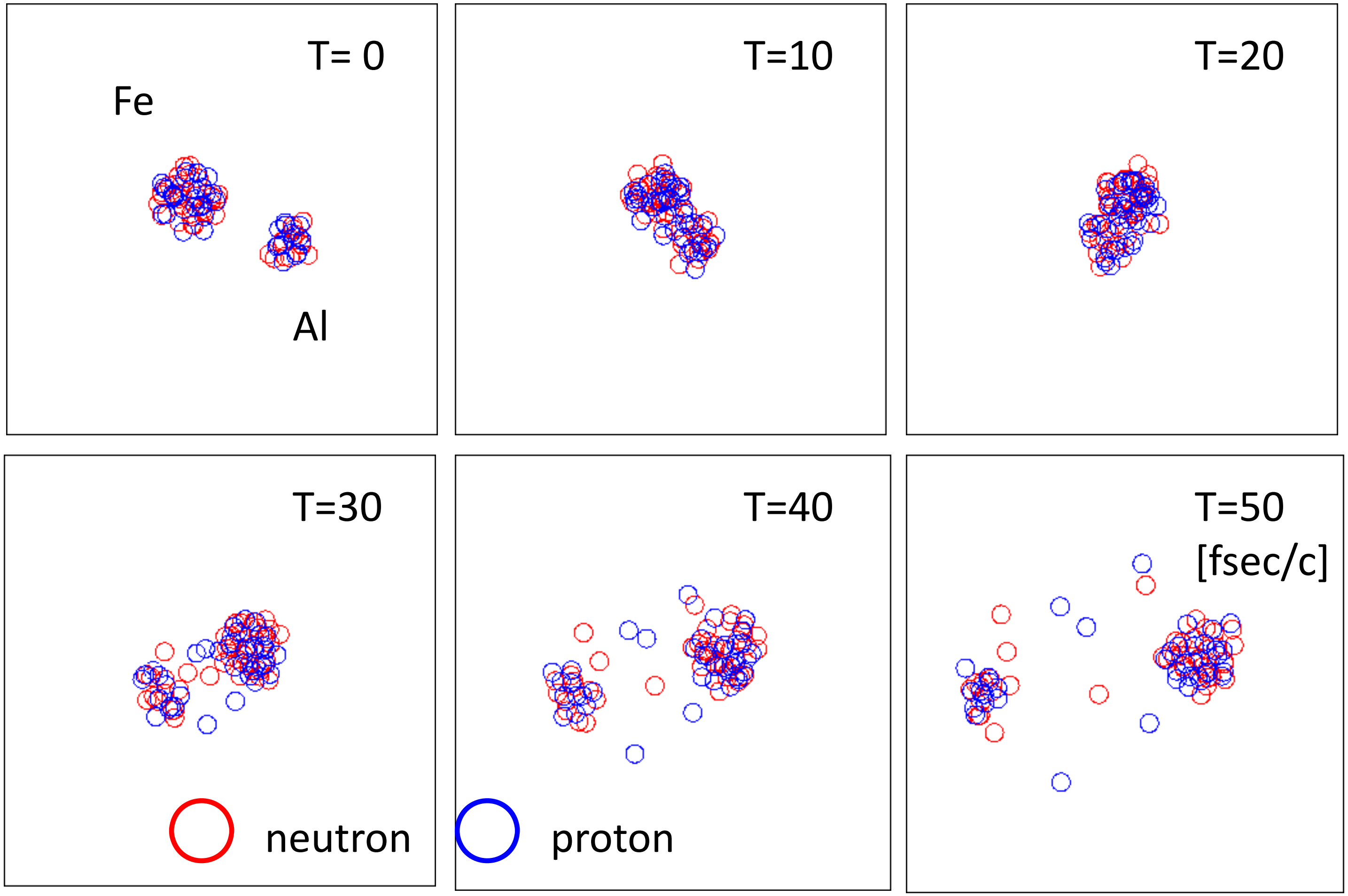
G4QMD(2)

- Time step of evolution in MD calculation is 1 fm/c and maximum number of time steps is 100. User can change both numbers from physics list.
- When positions of two particles close enough then scattering library is called and then final states of the scatter are checked in MD system to keep total energy of the system.
- After MD calculation, nucleons are grouped by their position and momentum (r = 4 fm and p = 0.1 GeV/c).
- Each group of nucleons is interpreted as an excited nucleus and its group momentum(CM motion), angular momentum and excited energy is calculated
- After that the excited nuclei are passed to Evaporation Models of Geant4
  - Recent Developments in Pre-equilibrium and De-excitation Models in Geant4, José M. QUESADA et al. (Oct21st, Session Index=J2)

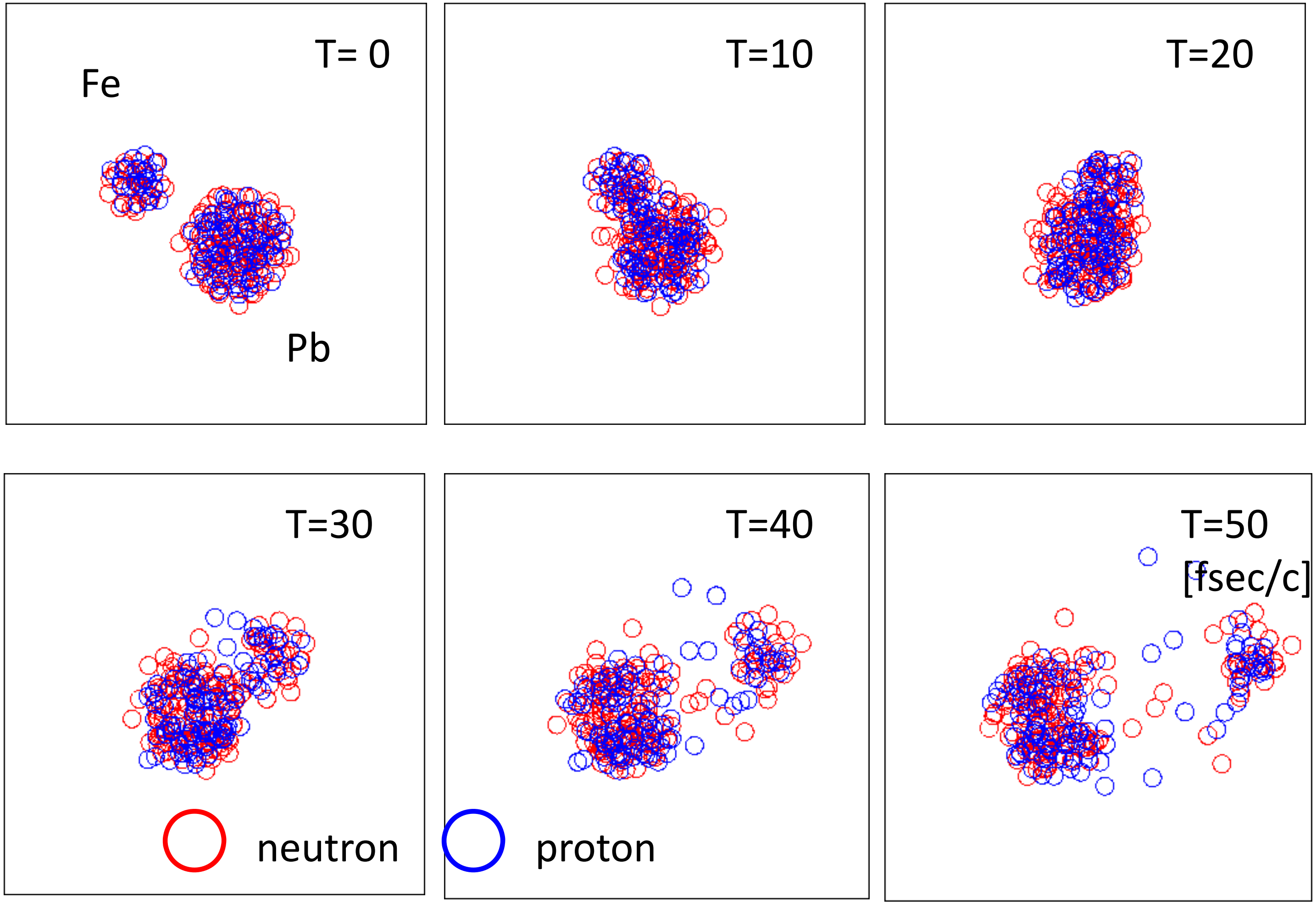
Collaboration Diagram



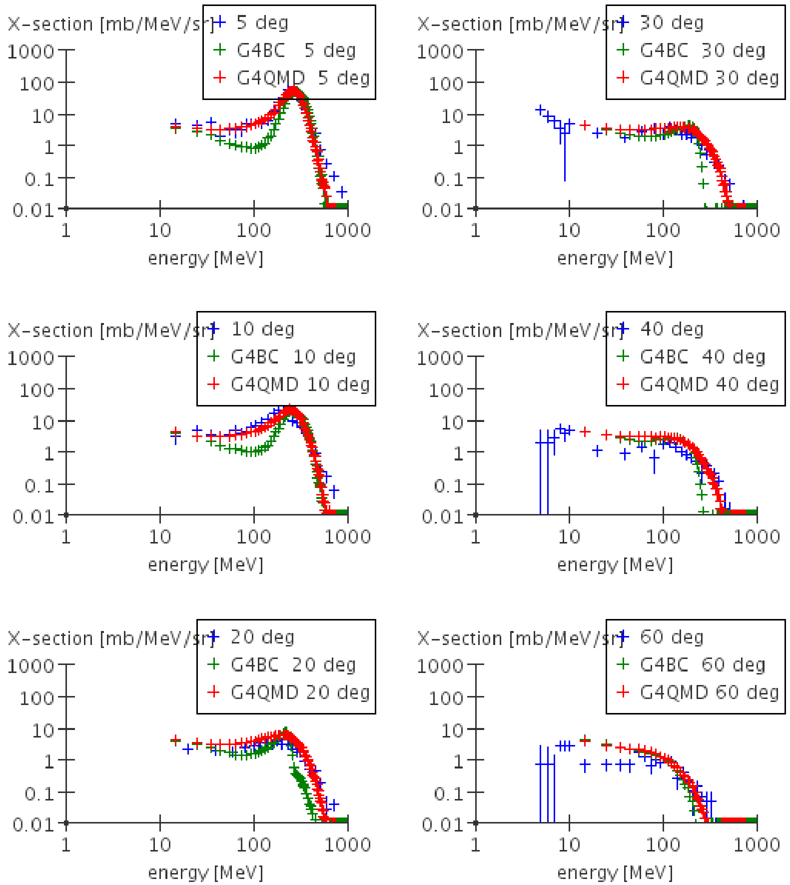
QMD Calculation
Fe 290MeV/n on Al



QMD Calculation
Fe 290MeV/n on Pb



C12 290MeV/n on Carbon
Secondary neutron spectra



+ Data *Iwata* et al., Phys. Rev. C64 (2001)

+ G4BinaryCascade

+ G4QMD

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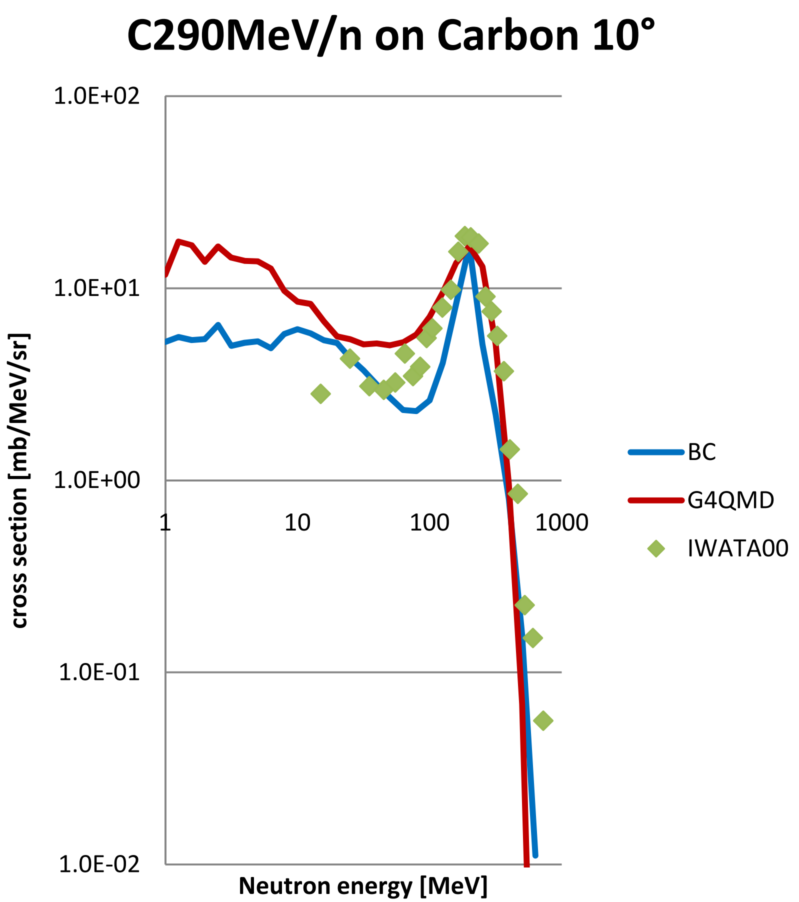
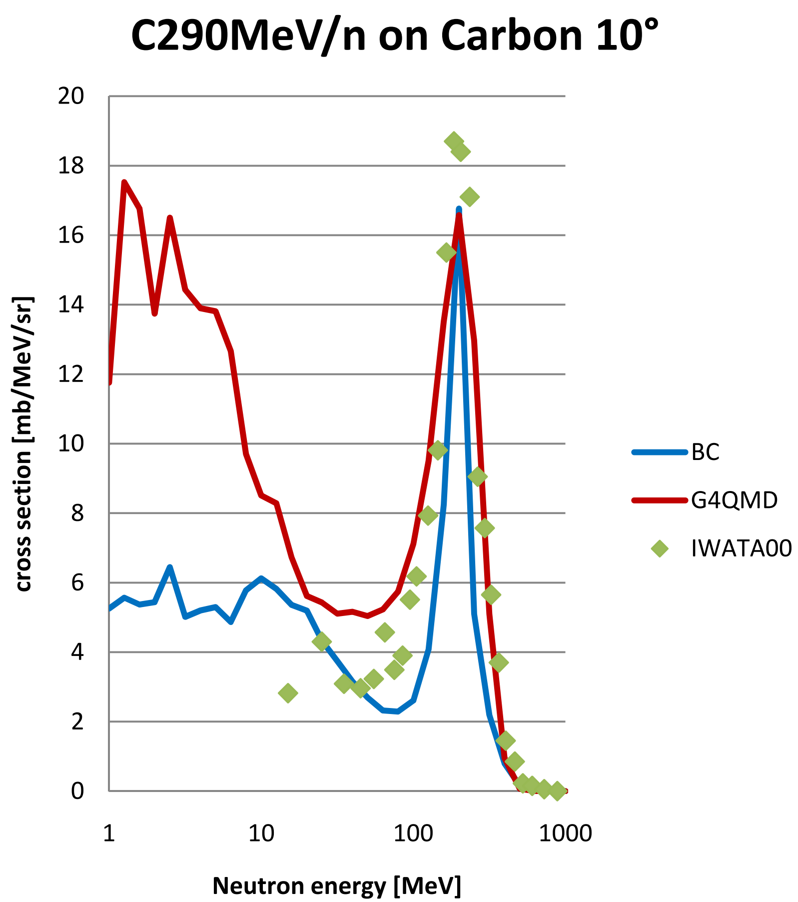
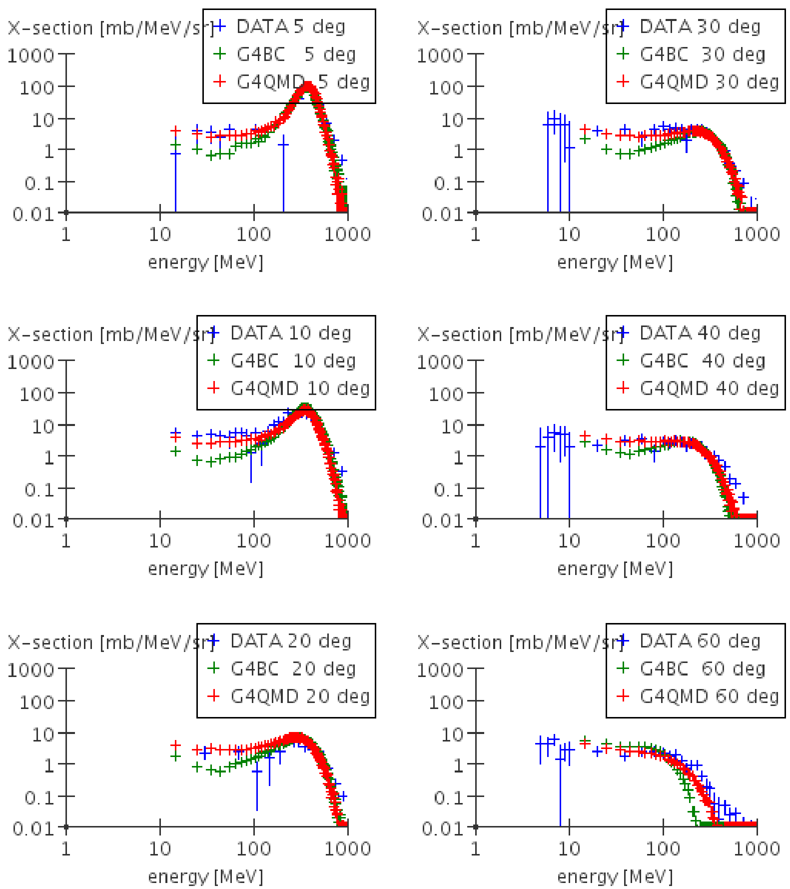




Ne20 400MeV/n on Carbon
Secondary neutron spectra



+ Data *Iwata* et al., Phys. Rev. C64 (2001)
+ G4BinaryCascade
+ G4QMD

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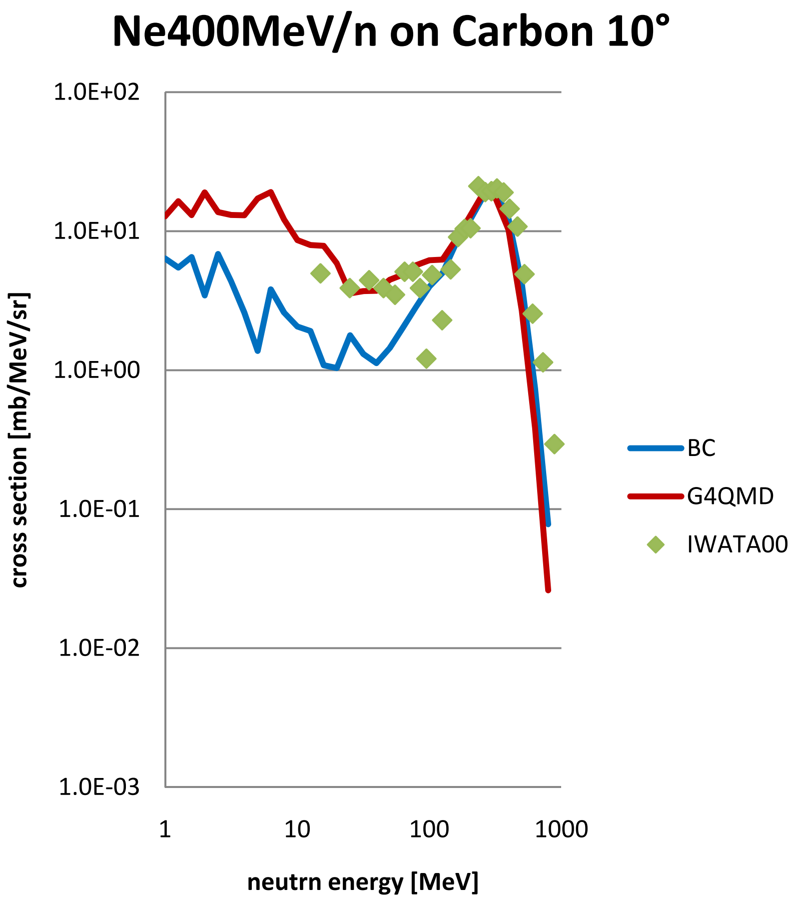
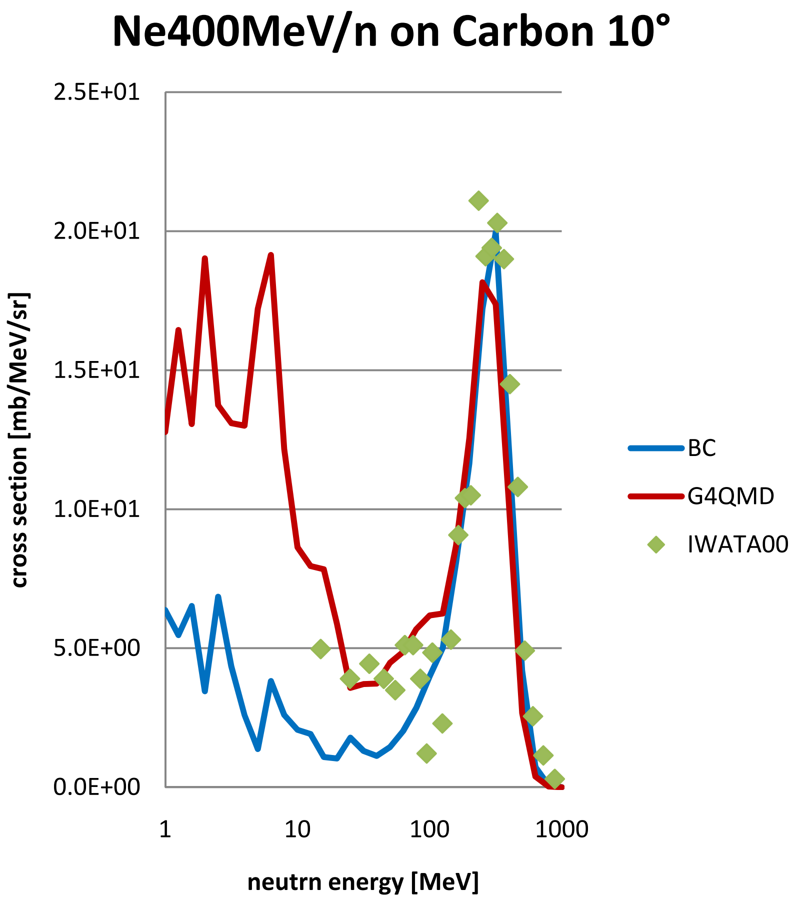
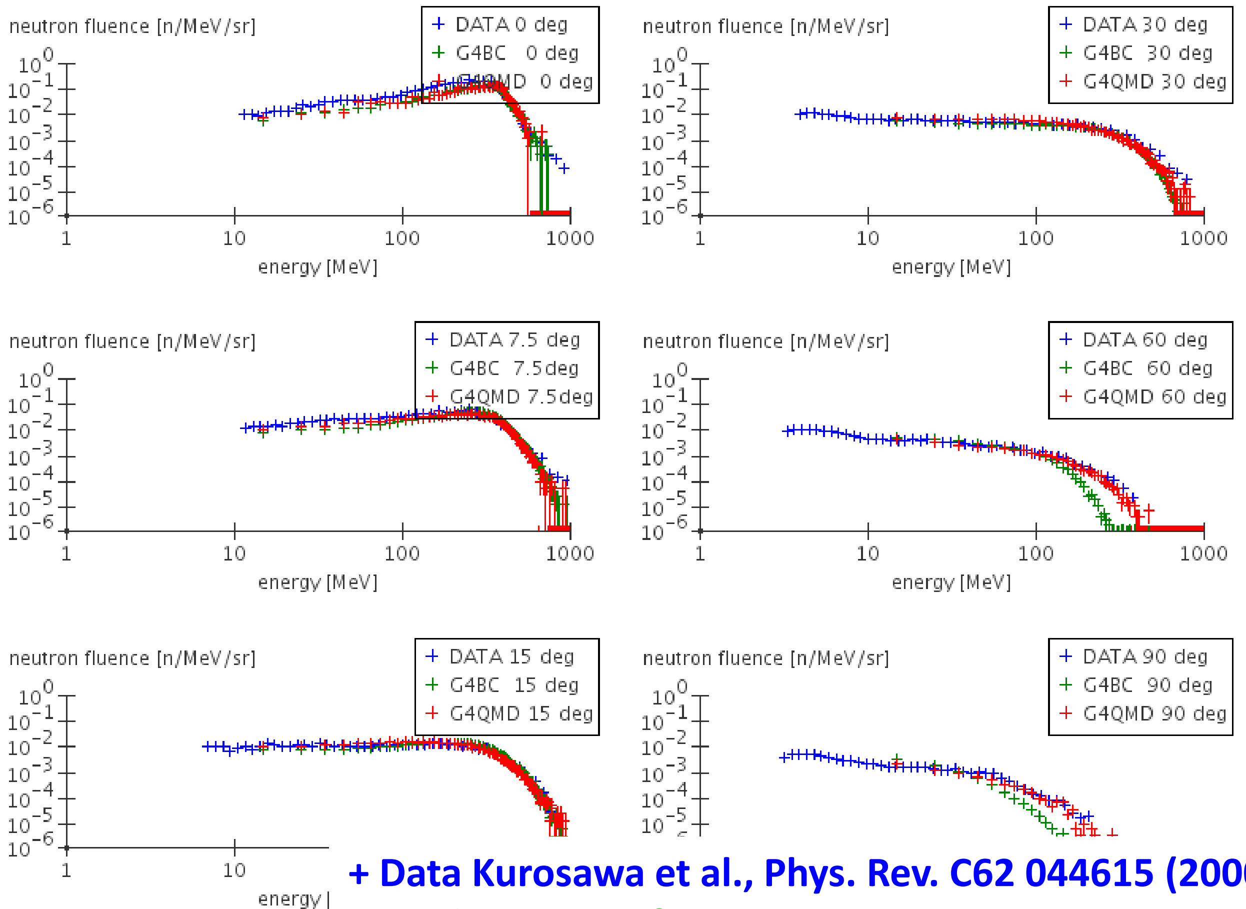




Fe56 400MeV/n on Thick Aluminum Neutron Yield



+ Data Kurosawa et al., Phys. Rev. C62 044615 (2000) ,
+ G4BinaryCascade, + G4QMD

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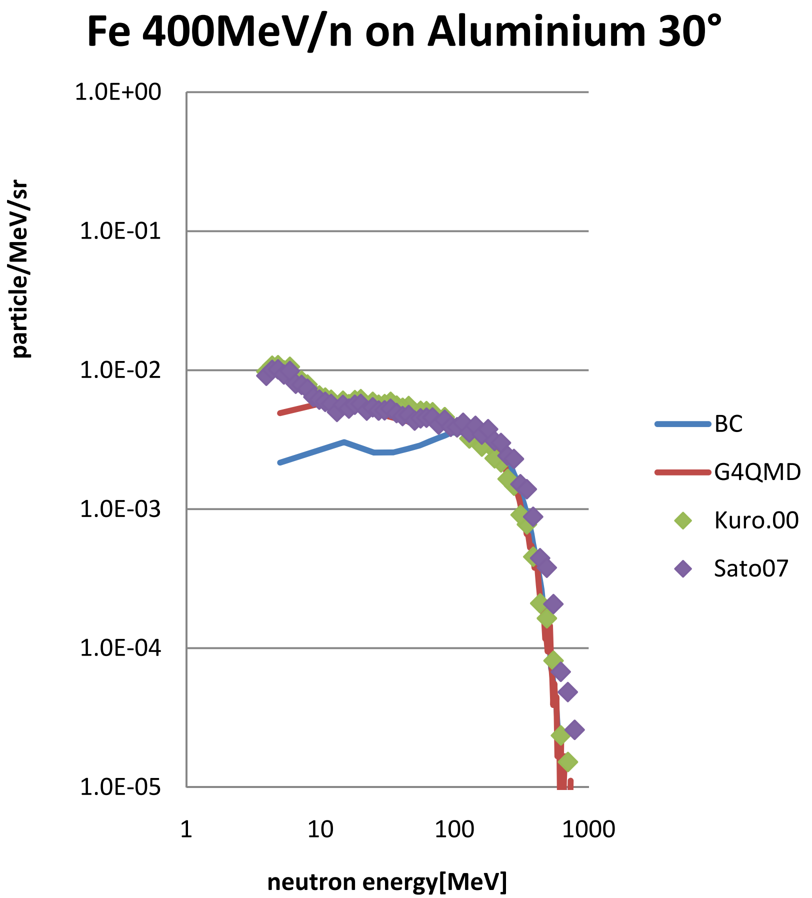
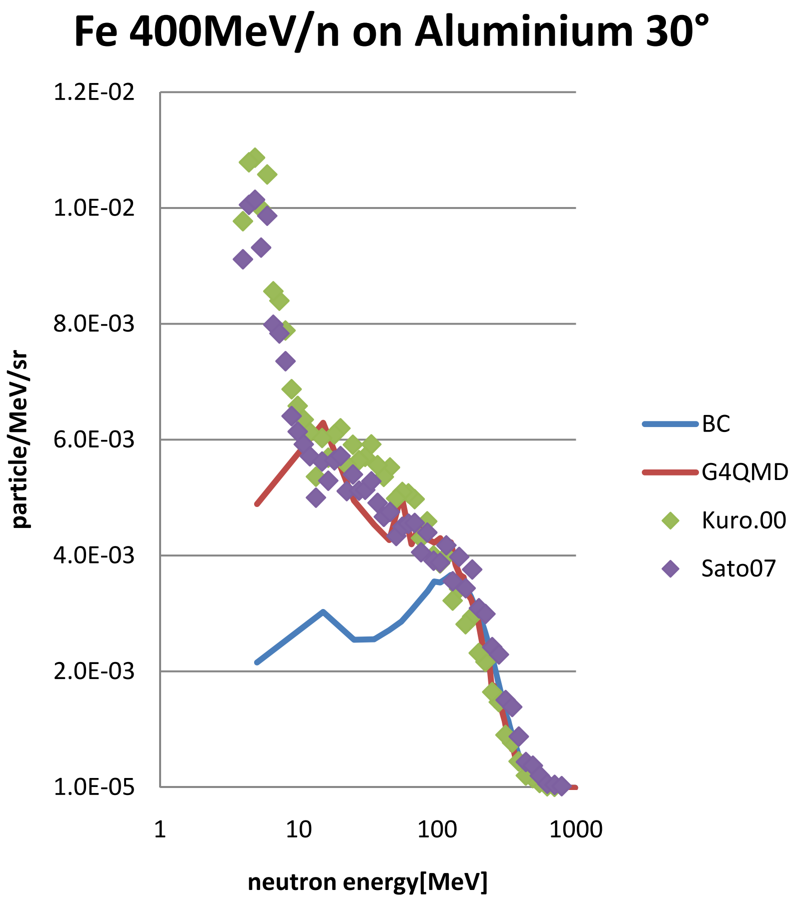
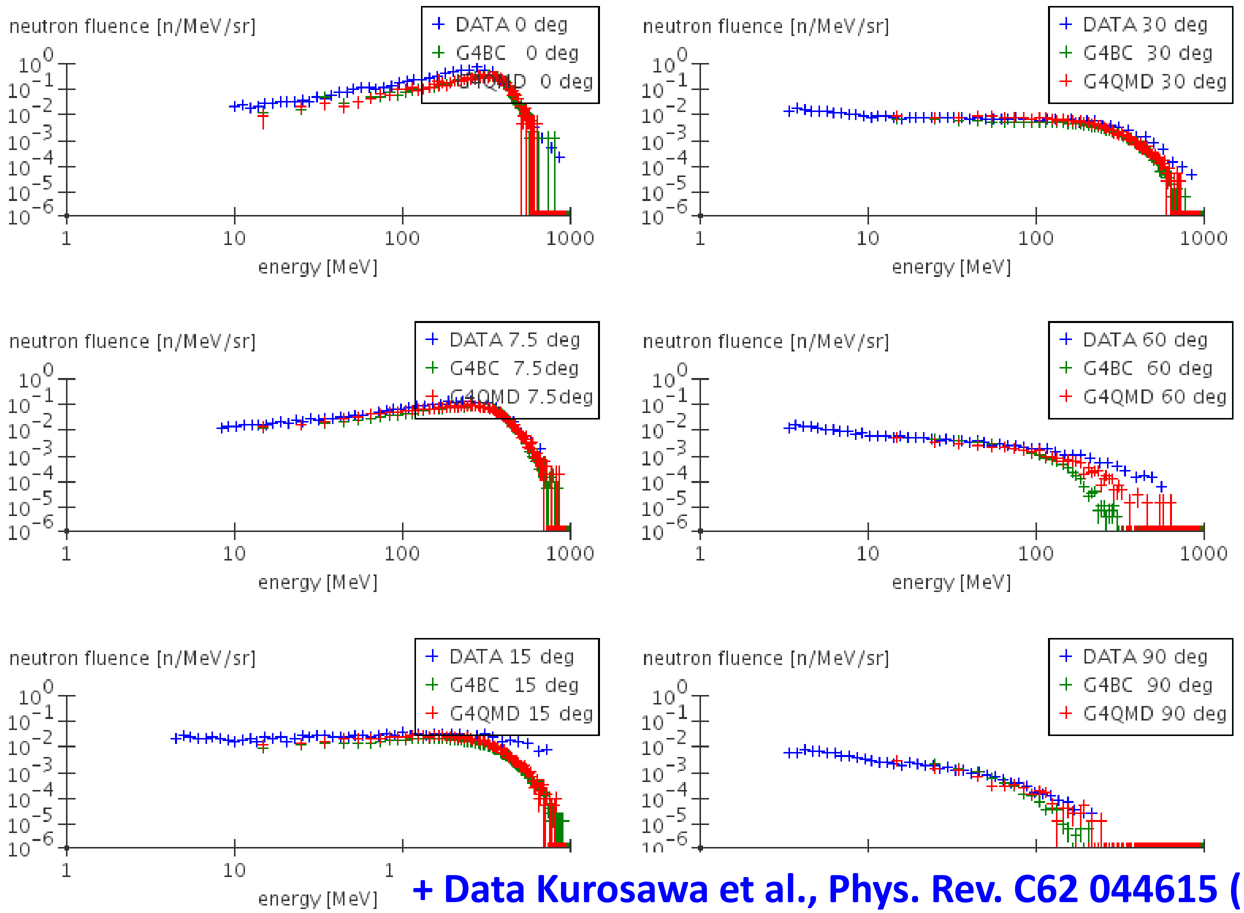




Sato 07 , Sato et al., J,NIM/A,583,507,2007

Xe132 400MeV/n on Thick Aluminum Neutron Yield



+ Data Kurosawa et al., Phys. Rev. C62 044615 (2000),
+ G4BinaryCascade, + G4QMD

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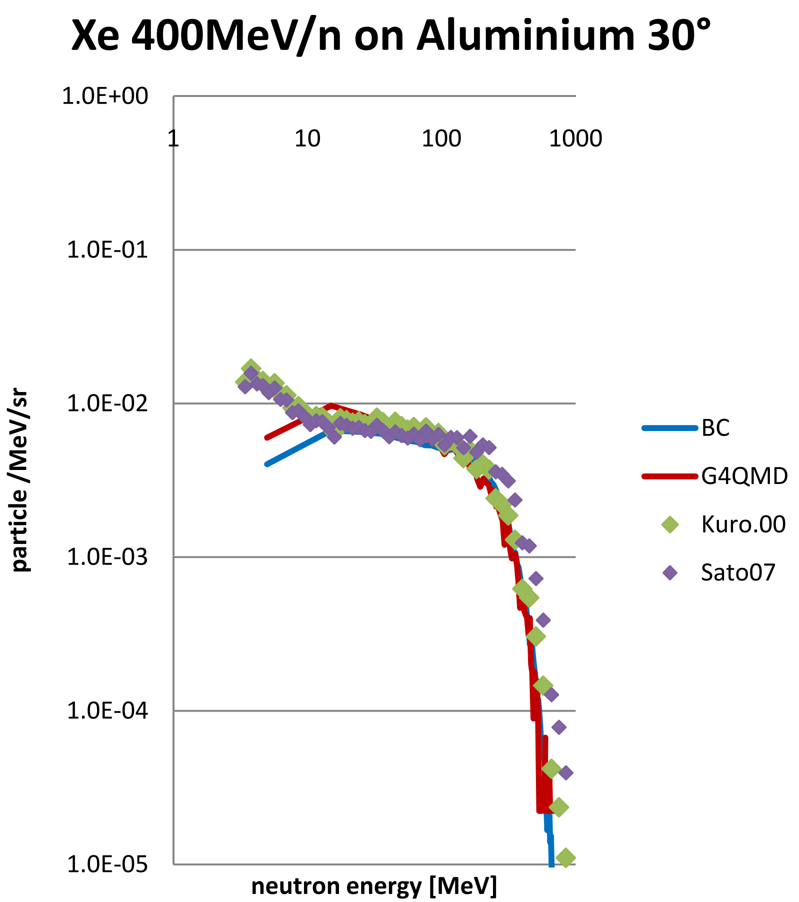
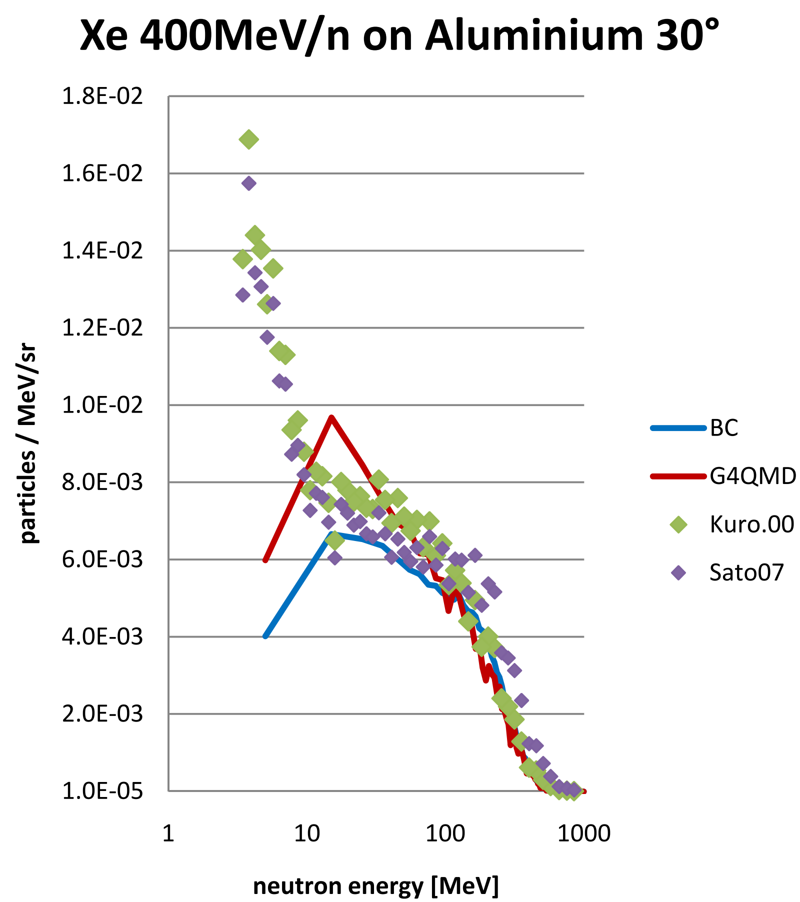




Lorentz covariant dynamics approach (1)

- Should be considered at relativistic energies
- Sorge et al. formulated Relativistic QMD in fully covariant way based on Poincaré-invariant constrained Hamiltonian dynamics.
- 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 (global 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 (2)

- 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 (3)

- 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

Lorentz covariant dynamics approach (4)

- However, recently developer of JQMD group published a new paper
- "In high-energy reactions, two-body collisions are dominant; the purpose of the Lorentz-covariant formalism is only to describe relatively low-energy phenomena between particles in a fast-moving medium. Therefore, we assume a simpler form for the time fixations, namely we set the time coordinates of all the particles to be the same. "

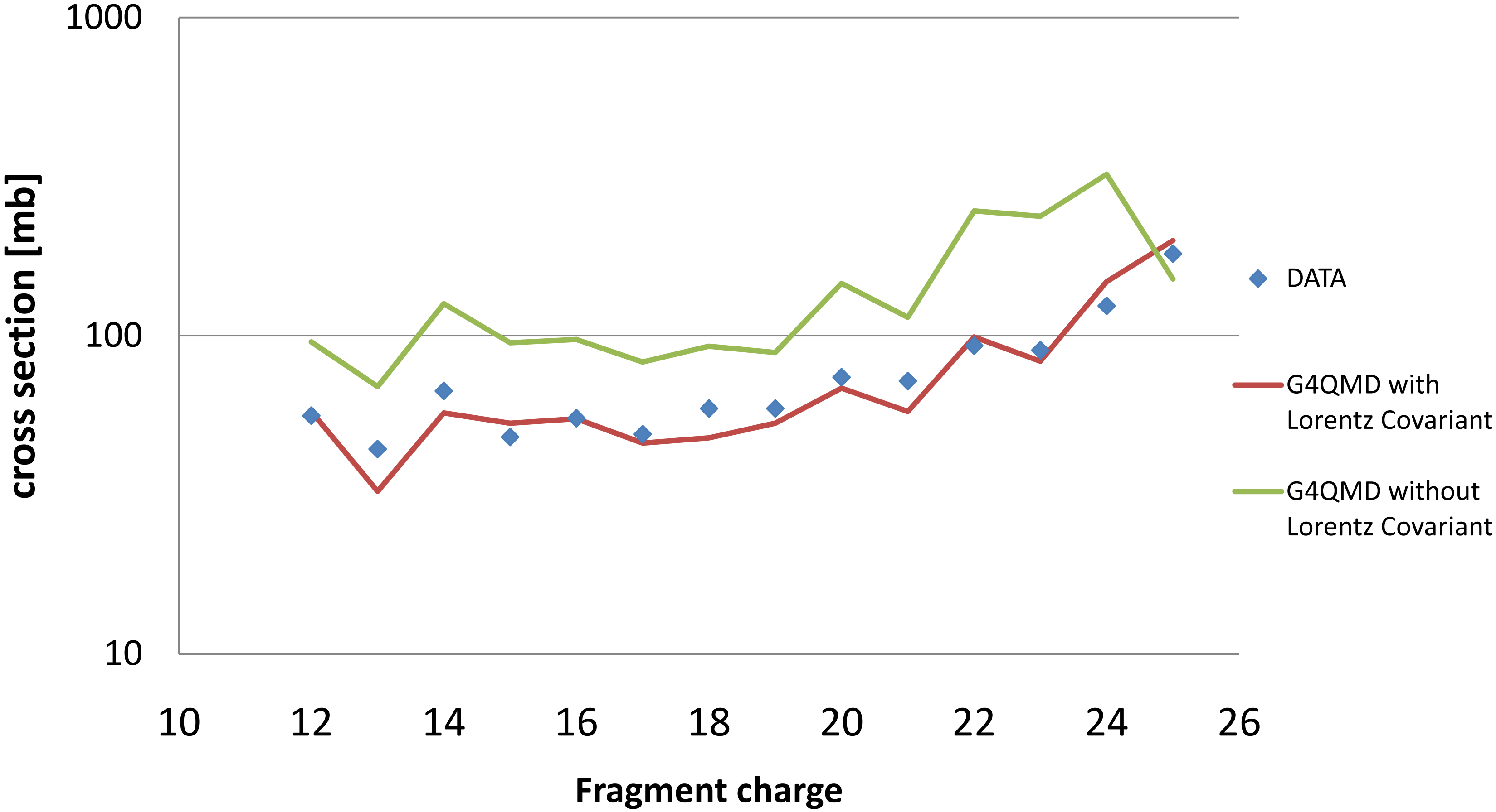
$$\phi_{i+N} \equiv a \cdot (q_i - q_N) \quad (i = 1,2,,,,N-1)$$

$$\phi_{2N} \equiv a \cdot q_N - t$$

- the inverted matrix S is not required.

D. Mancusiet al., "Stability of nuclei in peripheral collisions in the JAERI quantum molecular dynamics model" **PHYSICAL REVIEW C 79, 014614 (2009)**

Fe 1GeV/n on Al



Zeitlin et al., *Phys. Rev.* C **56**, 388-397 (1997)

Summary

- We are developing G4QMD which handles nucleus-nucleus interaction up to ~5 GeV/n
- Validation shows much better results than Binary (Light Ion) Cascade
- The first release was done in Geant4 v9.1
- We are also developing G4RQMD which has Lorentz covariant dynamics based on recent paper published by JQMD group.
- First validation of G4RQMD shows quite promising results in relativistic energy collisions and will be included in the coming Geant4 release.

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

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