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#### Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions

4 - 8 February 2008

Nuclear Reaction Models (JAM and JQMD) in PHITS

Koji Niita *RIST* Ibaraki Japan

## Reaction Models (JAM and JQMD) in Particle and Heavy Ion Transport code System

# PHITS

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## Contents

- (1) Overview of PHITS
- (2) Application Fields of PHITS
- (3) Reaction Models (JAM and JQMD) in PHITS
- (4) Strategy for better description of Nuclear Reactions

## **PHITS : Particle and Heavy Ion Transport code System**

PHITS is a multi-purpose 3D Monte Carlo transport code system for all particles and Heavy ions with all energies from meV up to 200 GeV.

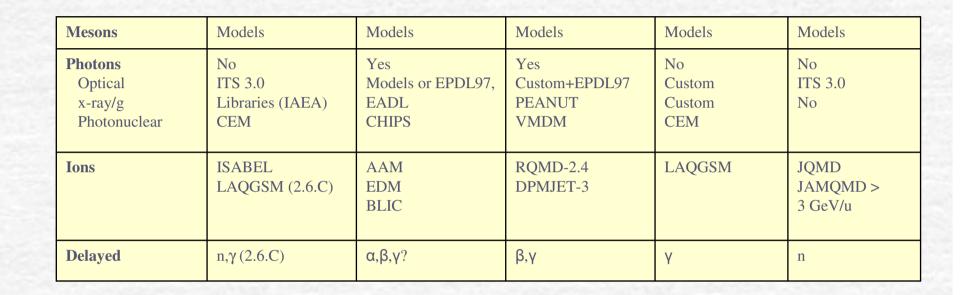
	MCNPX	GEANT4	FLUKA	MARS	PHITS
Lab. Affiliation	LANL	CERN,IN2P3 INFN,KEK,ESA, SLAC,TRIUMF	CERN INFN	FNAL	JAEA,RIST GSI,KEK Chalmers Univ.
Language	Fortran 90/C	C++	Fortran 77	Fortran 95/C	Fortran 77
Release Format	Source & binary	Source & binary	Source & binary	Binary	Source & binary
Users	~2000	~1000	~1000	220	220
Parallel Exec.	Yes	Yes	No	Yes	Yes

5 major codes for all particle transport in a world

By G. W. McKinney in FNDA (Fast Neutron Detectors and Applications Conference) April 2006 Revised by L. Waters in HSS06 (Hadronic Shower Simulation Workshop) Sep. 2006

## **Physics Capabilities**

Physics	MCNPX	GEANT4	FLUKA	MARS	PHITS
Particles	34	68	68	41	38
Charged particles Energy loss Scatter Straggling XTR/Cheren.	CSDA Bethe-Bloch Rossi Vavilov No	CSDA Bethe-Bloch Lewis Urban Yes	CSDA Bethe-Bloch Moliere improved Custom No/yes	CSDA Bethe-Bloch Moliere improved Custom No	CSDA Bethe-Bloch Moliere Vavilov No
Baryons Neutron Low High Proton Low High Other	Cont. (ENDF) Models Cont. (ENDF) Models Model List: Bertini ISABEL CEM INCL FLUKA89>3 GeV LAQGSM (2.6.C)	Cont. (ENDF) Models Models Model list: Hadron-nucleous GHEISHA* INUCL(Bertini) BIC CHIPS QGS/FTF>8 GeV	Multigroup(72) Models Models Model list: PEANUT(GINC) +DPM+Glauber	Cont. (ENDF) Models Models Model list: Custom CEM LAQGSM DPMJET	Cont. (ENDF) Models Models Model list: Bertini JAM>3 GeV
Leptons Electrons	ITS 3.0	Models/EEDL, EADL	Custom	Custom	ITS 3.0
Muon Neutrino Other	CSDA/decay Production Decay	Models Production Decay	Models Models Decay	Models Models Models	CSDA/decay Models Models



## **Overview of PHITS** (Particle and Heavy Ion Transport code System)



#### PHITS = MCNP + JAM + JQMD

ſ	MCNP	Neutron, Photon, Electron Transport by Nuclear Data
-	JAM	Hadron-Nucleus Collisions up to 200 GeV
	JQMD	Nucleus-Nucleus Collisions by Molecular Dynamics

**External Field:** Magnetic Field, Gravity Optical and Mechanical devices

#### Language and Parallelism

FORTRAN 77

#### **Transport Particle and Energy**

(	Proton	0 ~ 200 GeV
	Neutron	10 <sup>-5</sup> eV ~ 200 GeV
	Meson	0 ~ 200 GeV
	Barion	0 ~ 200 GeV
	Nucleus	0 ~ 100 GeV/u
	Photon	1 keV ~ 1 GeV
	Electron	1 keV ~ 1 GeV

Geometry: CG and GG

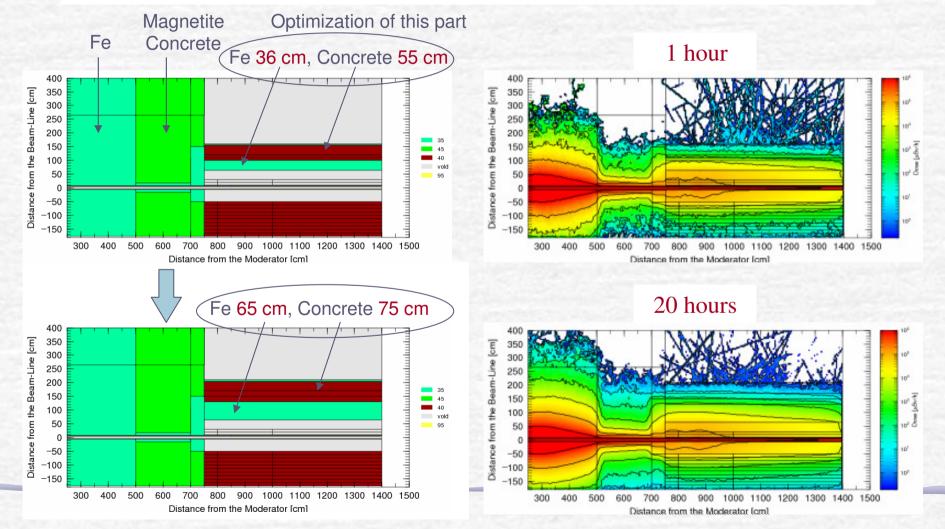
#### Tally, Mesh and Graphic

Tally: Track, Cross, Heat, Star, Time, DPA, Product, LET Mesh: cell, r-z, xyz Counter: Graphic: ANGEL (PS generator)

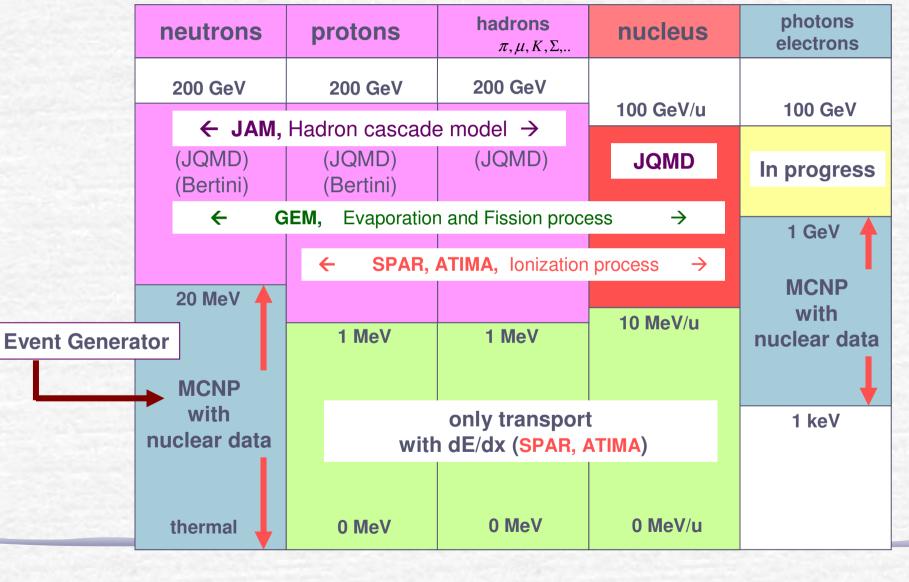
**PHITS**: H. Iwase et.al. J. Nucl. Sci. Technol. **39** (2002) 1142

## User Interfaces of **PHITS**

**2D** output of the **intermediate results** of a certain interval of histories. This function is very powerful for optimization study **!!!** 



#### Map of Models, transport particles and energies in PHITS



#### What are we doing in Monte Carlo calculations for particle transport ?

 Solving one-body Boltzmann equation by using the evaluated nuclear data.

MCNP type code energy is conserved in average. no correlations

 Simulating real phenomena by using event generators.

• PHITS for high energy by JAM, JQMD. treat all ejectiles of collisions. energy and momentum are conserved in each collision.

Any observables

Only one-body observables

**Event Generator** 

Observables beyond one-body quantities are often required.

We have developed the event generator mode in PHITS for all energy.

## Event Generator Mode for low energy neutrons in **PHITS**

#### Neutron data + Special Evaporation Model

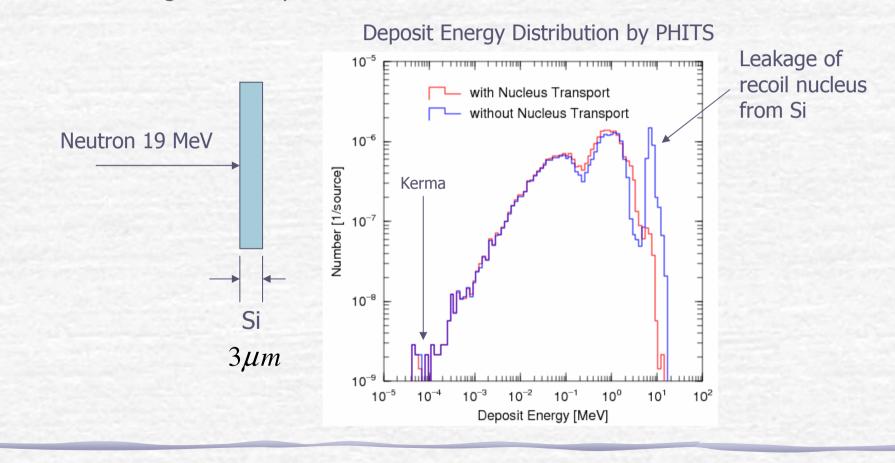
We use the channel cross sections and neutron energy spectrum of the first neutron and assume the binary decay of recoiled nucleus.

Neutron<br/>channelscapture<br/> $\Gamma_n = 0$ charged particle and photon decay<br/>final state is uniquely determined<br/>charged particle and photon decay<br/>after the first neutron emissionNeutron<br/>(n,n') $\Gamma_n = 0$ charged particle and photon decay<br/>after the first neutron emission

By this model, we can determine all ejectiles (neutrons, charged particles, nucleus and photons) with keeping energy and momentum conservation.

PHITS can transport all charged particle and nucleus down to zero energy and estimate deposit energy without local approximation (kerma factor). An example of Event Generator Mode

Neutron-induced semiconductor soft error SEU: single event upset



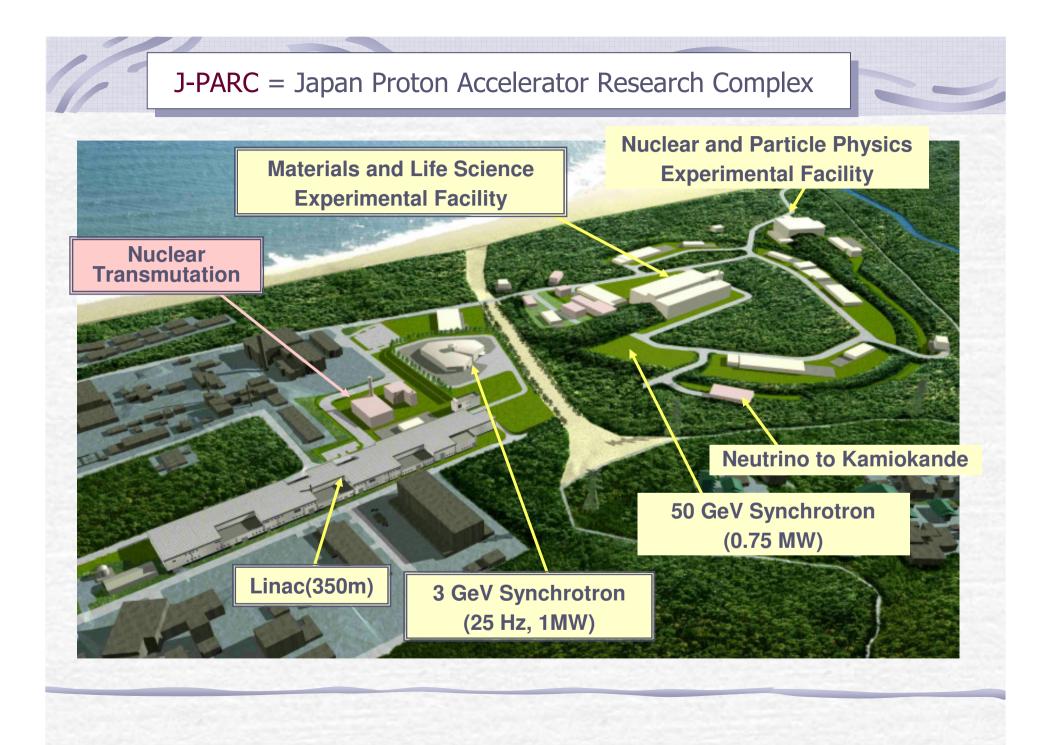
**Event Generator Mode** 

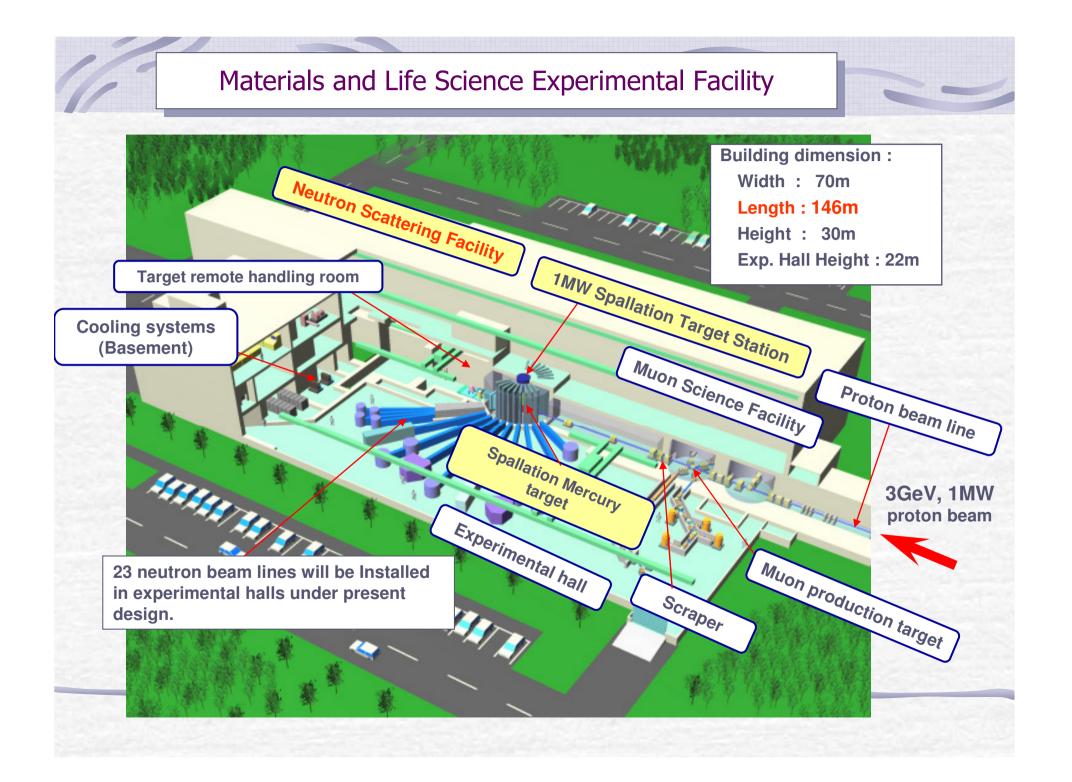
**Application Fields of PHITS** 



J-PARC Spallation Neutron Source Neutron Optics Heavy Ion Facilities

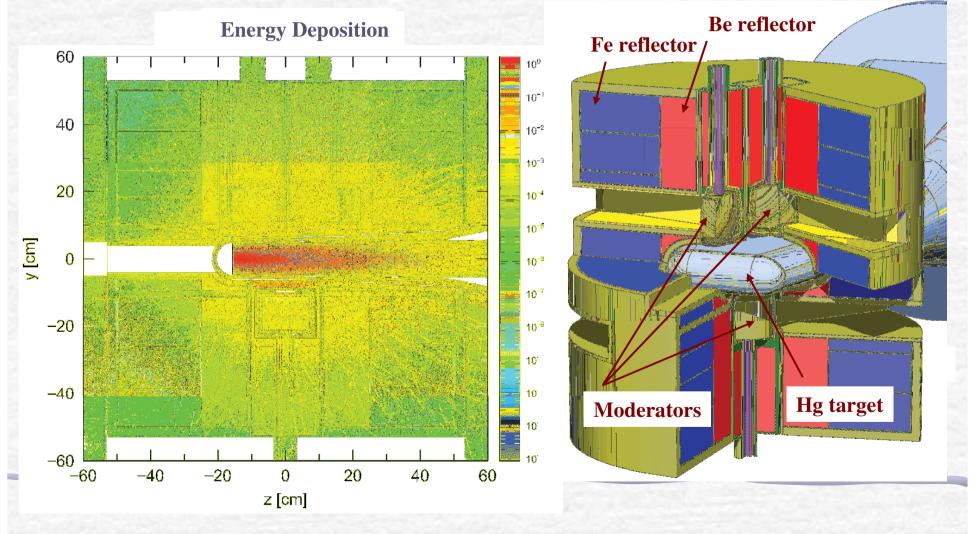
BNCT Proton and Heavy Ion Therapy Dose in Space Shuttle Atmospheric Cosmic-Ray



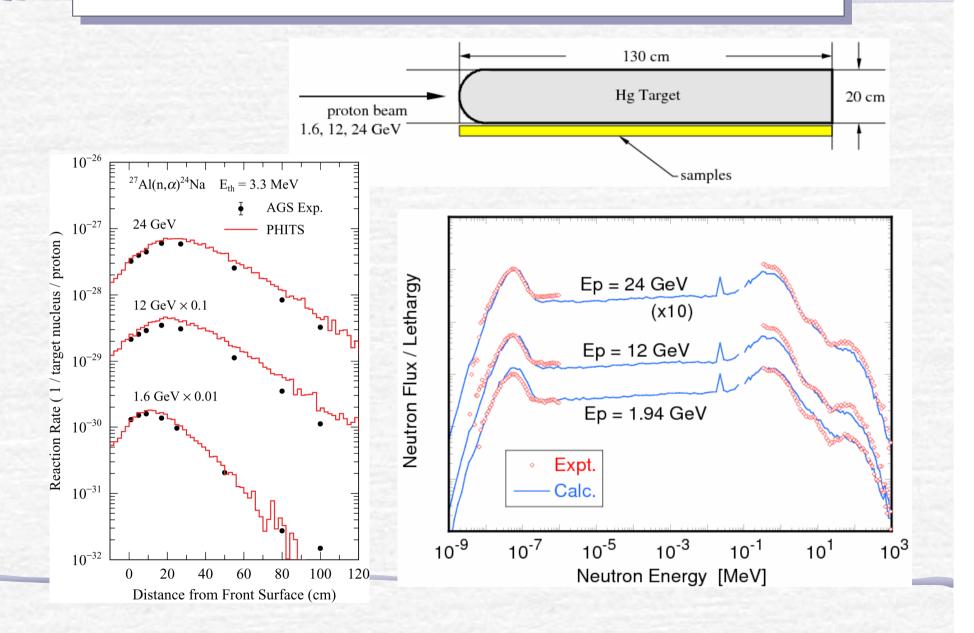


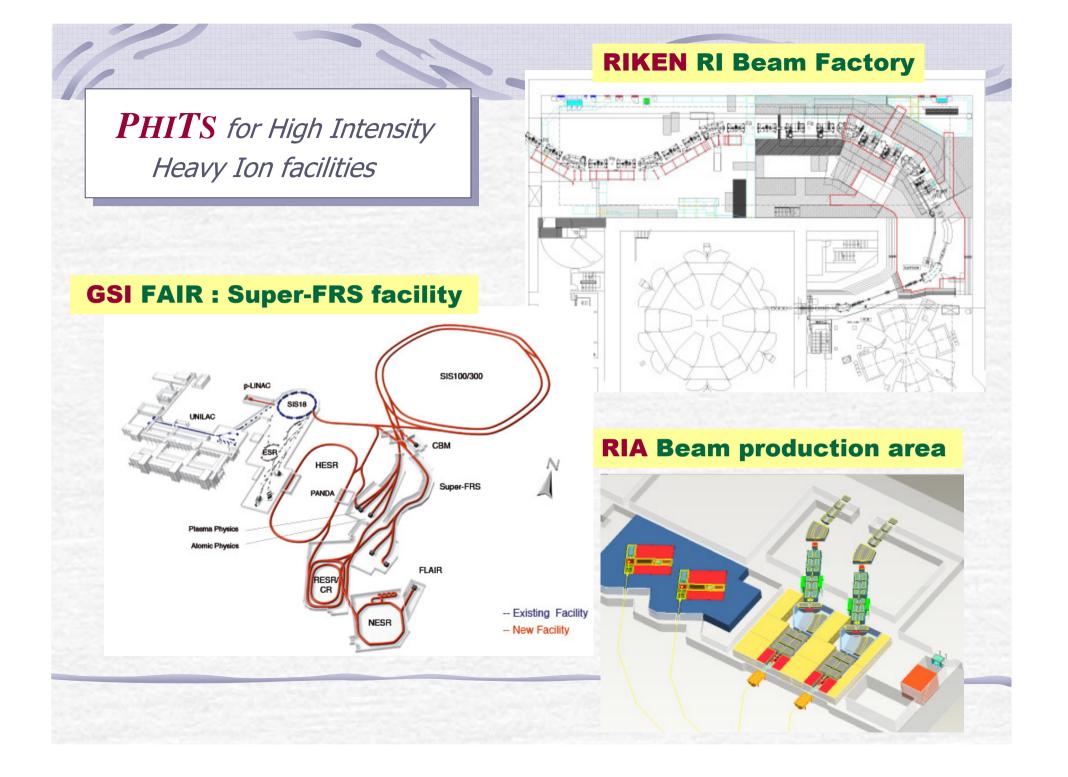
#### Spallation Neutron Source in Proton Accelerator Facilities

PHITS has been extensively used for Optimization and Shielding design around Hg target of J-PARC



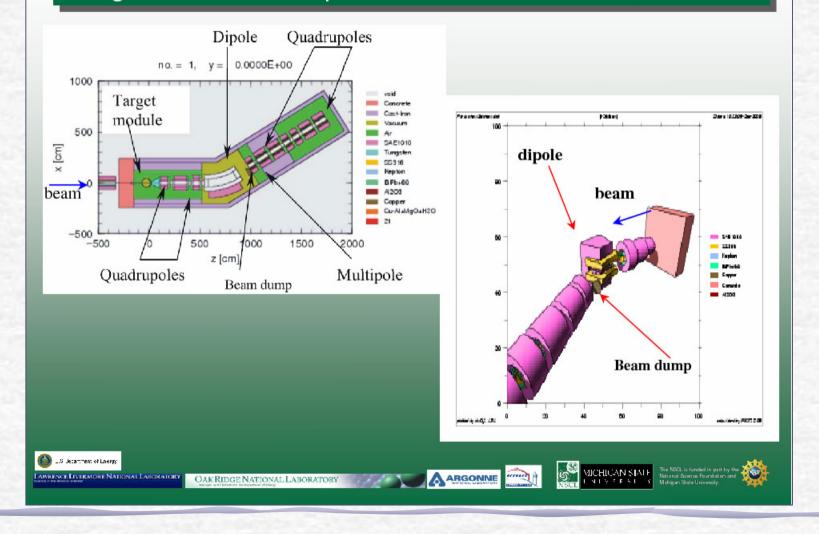
### AGS Benchmark Experiments for Spallation Neutron Source



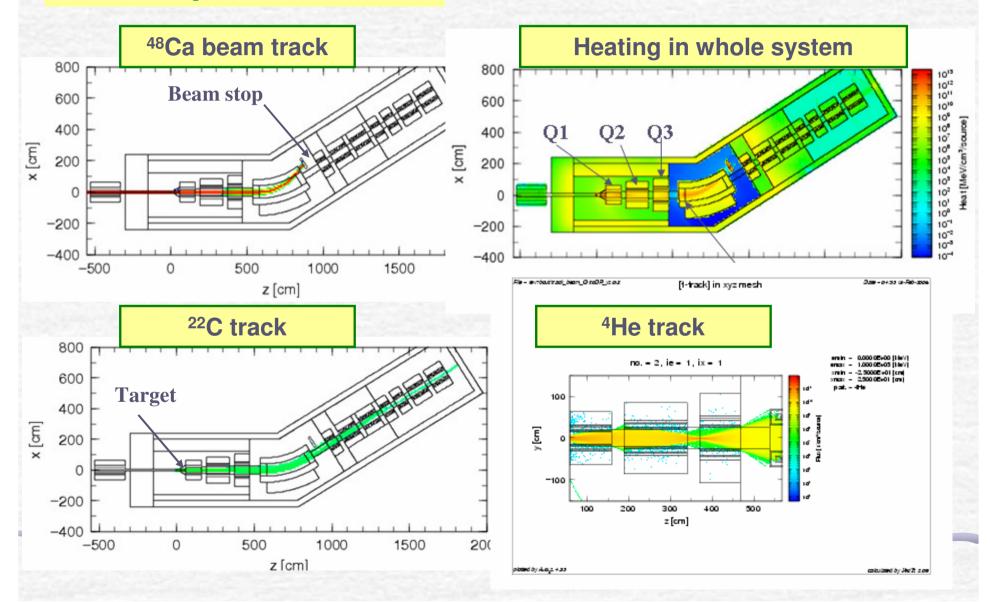


R.M. Ronningen presentation at Hadronic Shower Simulation Workshop FNAL September 6-8, 2006

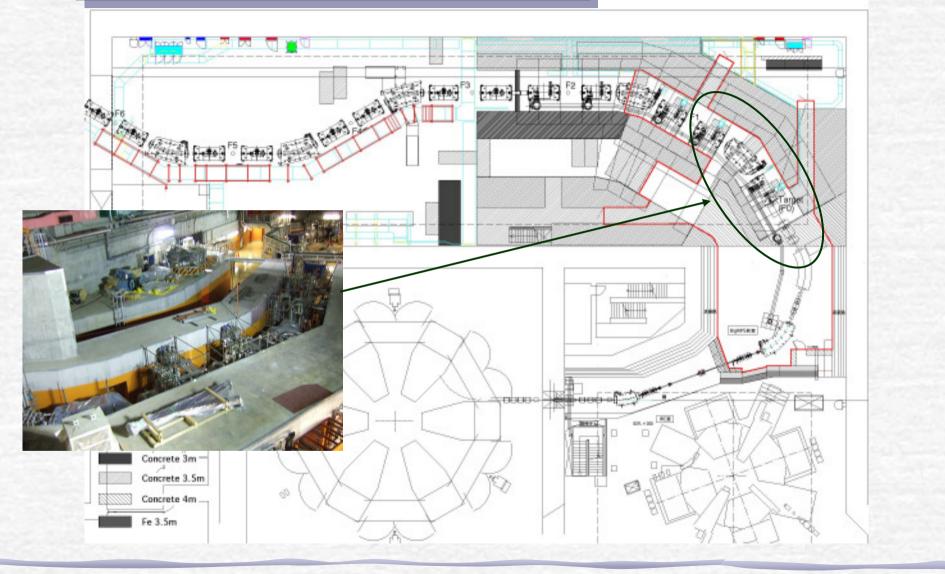
#### Fragmentation Pre-Separator in PHITS (Inseok Baek, NSCL/MSU)



**RIA Beam production area** 



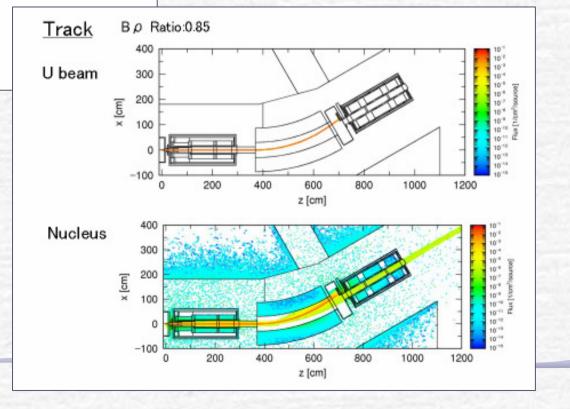
#### **RIKEN RIBF: RI Beam Factory**

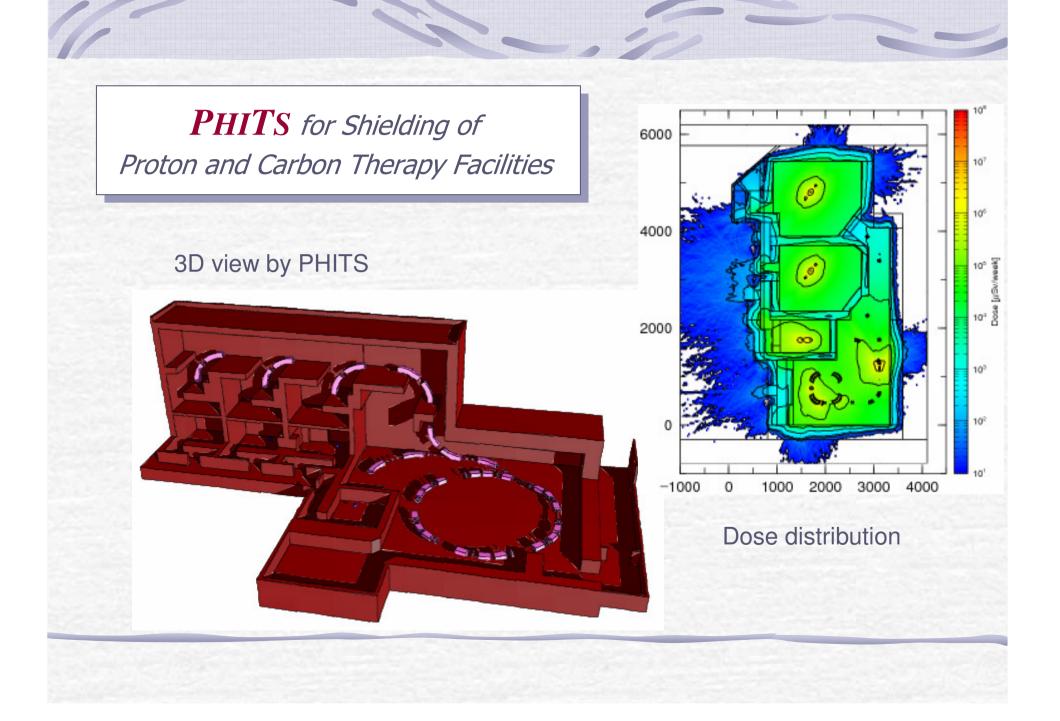


#### PHITS Simulation for BigRIPS

2006/5 Expert-Meeting at RIKEN <u>BigRIPS</u> Team

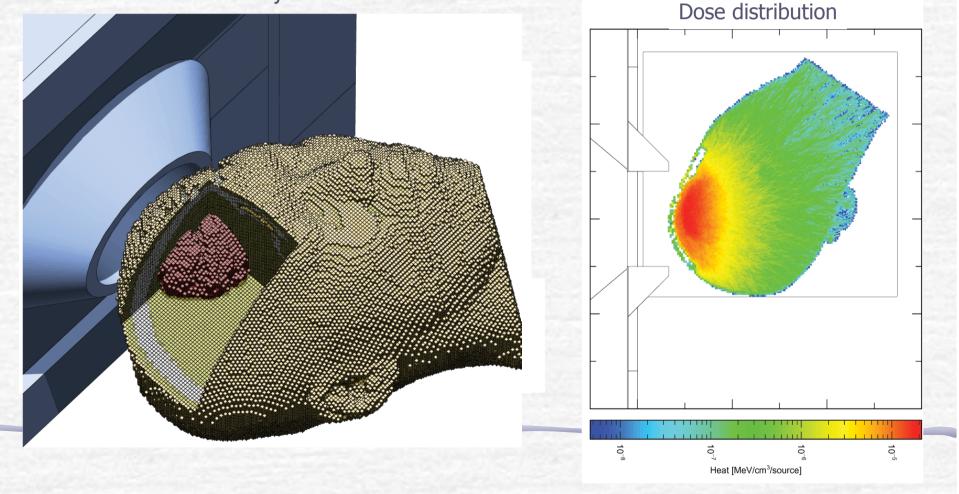
- 1. Heat load
- 2. Radiation damage
- 3. DPA

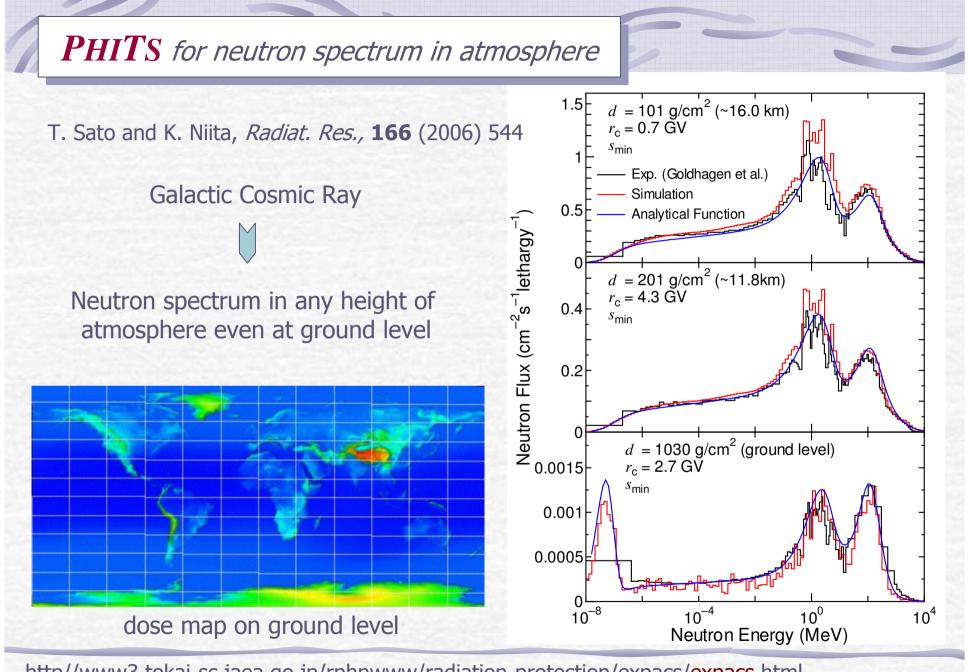




**PHITS** for planning system for radiotherapy

**Boron Neutron Capture Therapy at Dept. Research Reactor, JAERI** 3D view by PHITS **JCDS** (Jaeri Computational Dosimetry System) creates the Voxel data from CT and MRI data for MCNP (PHITS ) calculation.





http//www3.tokai-sc.jaea.go.jp/rphpwww/radiation-protection/expacs/expacs.html

JENDL High Energy File 2007 JENDL/HE-2007 neutron and proton ~ 3GeV, 106 nuclei

H-1, C-12,13, N-14, O-16, F-19, Na-23, Mg-24,25,26, Al-27, Si-28,29,30, Cl-35,37, Ar-36,38,40, K-39,41, Ca-40,42,43,44,46,48, Ti-46,47,48,49,50, V-51, Cr-50,52,53,54, Mn-55, Fe-54,56,57,58, Co-59, Ni-58,60,61,62,64, Cu-63,65, Zn-64,66,67,68,70, Ga-69,71, Ge-70,72,73,74,76, As-75, Zr-90,91,92,94,96, Nb-93, Mo-92,94,95,96,97,98,100, Ta-181, W-180,182,183,184,186, Au-197, Hg-196,198, 199,200,201,202,204, Pb-204,206,207,208, Bi-209, U-235,238, Np-237, Pu-238,239,240,241,242, Am-241,242,242m

http://wwwndc.tokai-sc.jaea.go.jp/ftpnd/jendl/jendl-he-2007.html

### **Physical Processes included in PHITS**

Transport between collisions **External Field** and Optical devices

Ionization process for charge particle Magnetic Field Gravity Super mirror (reflection) Mechanical devices, T0 chopper

#### SPAR, ATIMA code

Energy straggling Angle Straggling

Collisions with nucleus Nuclear Data ENDF-B/VI, LA150, ..... Particle Induced Collisions

Heavy Ion Collisions

MCNP code

JAM code

JQMD code

-Nuclear Reaction Models

**MCNP code** for Neutron Transport below 20 MeV with Nuclear Data

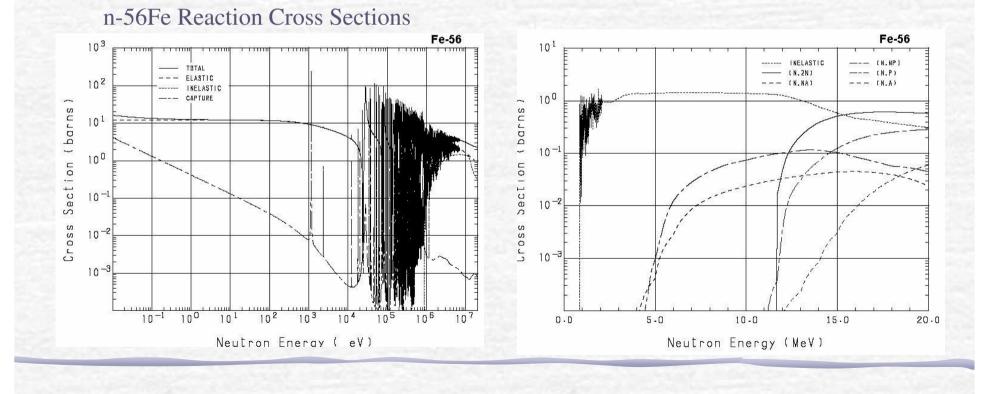
*Monte Carlo N-Particle Transport Code System* developed by Los Alamos National Lab.

for Neutrons, Photons, Electrons

by using Evaluated Nuclear Data, such as ENDF, JENDL, ...

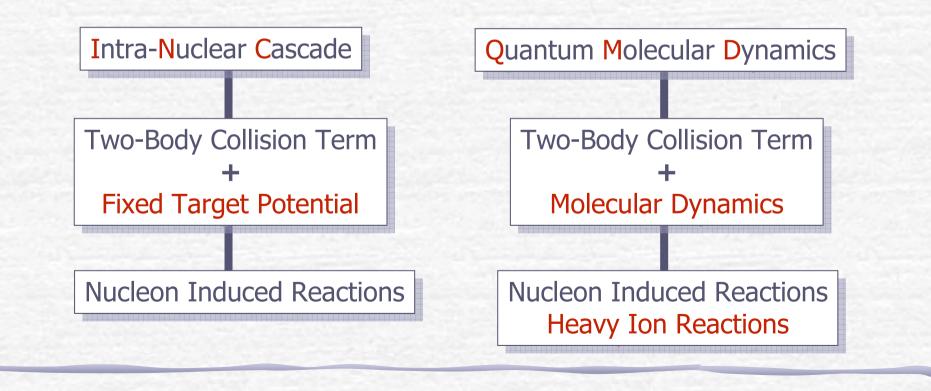
Applications:

Nuclear Criticality Safety, Radiation Shielding, Fission Reactor Design, ...



#### Numerical Simulation for high energy nuclear reactions

- 1. Tow-Body Collision (hard interaction)
  - elementary cross sections for hadrons
- 2. Potential (soft interaction)
  - ground state, residual nucleus, excitation energy, recoil energy

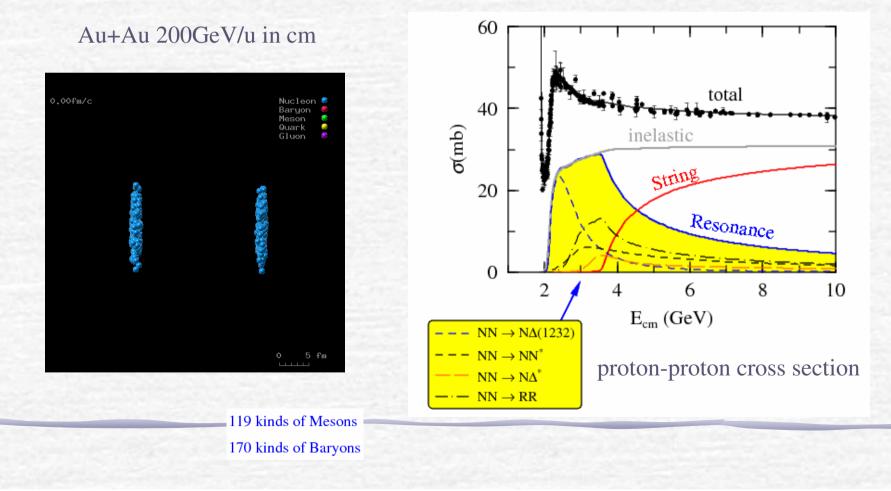


#### **JAM code** for Hadron Nucleus Collisions up to 200 GeV



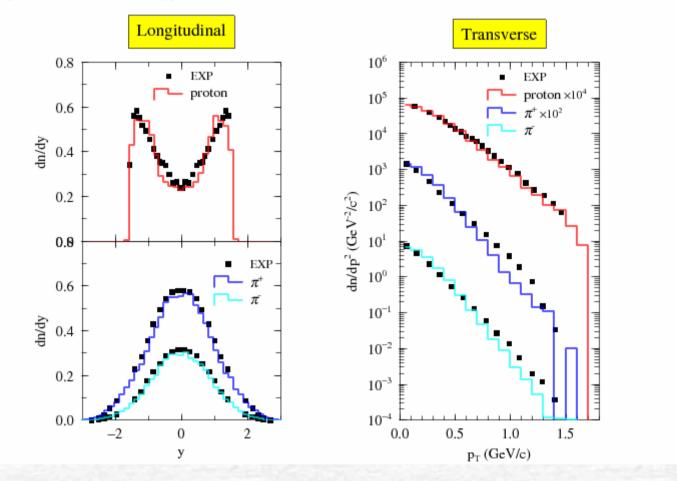
**Introducing JAM** (Jet AA Microscopic Transport Model) Y. Nara et.al. Phys. Rev. C61 (2000) 024901 JAM is a Hadronic Cascade Model, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles.

We have parameterized all *Hadron-Hadron Cross Sections*, based on *Resonance Model* and *String Model* by fitting the available experimental data.



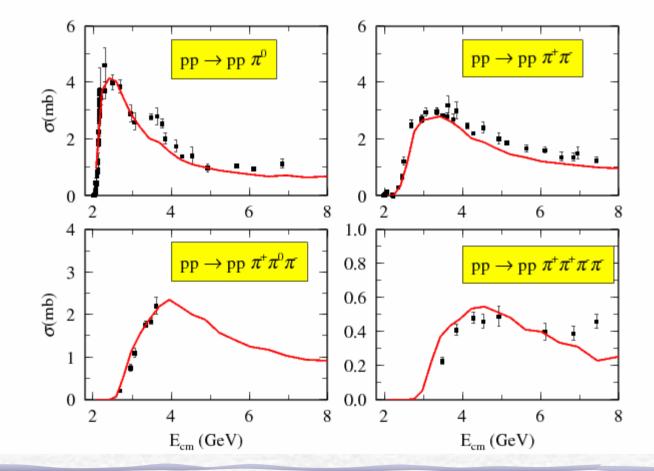
## Proton-Proton (12GeV/c) Inclusive Spectra

Rapidity y distributions (left panel) and the transverse momentum distributions (right panel) of proton,  $\pi^+$  and  $\pi^-$  in pp collisions at 12 GeV/c.



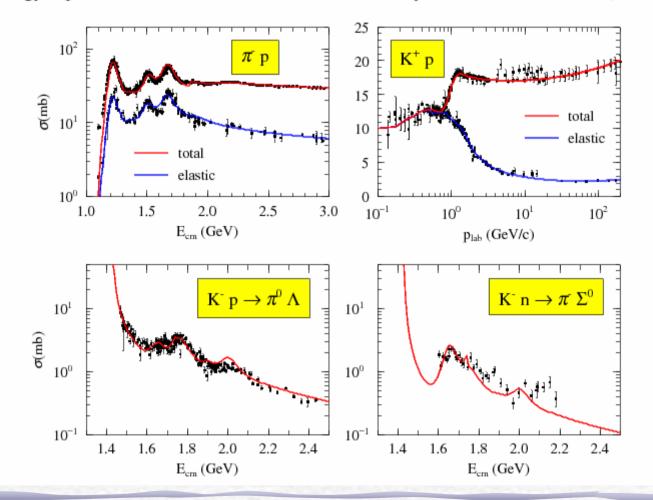
#### Proton-Proton Exclusive Cross Sections

Energy dependence of the exclusive pion production cross sections for proton-proton reactions as a function of c.m. energy.



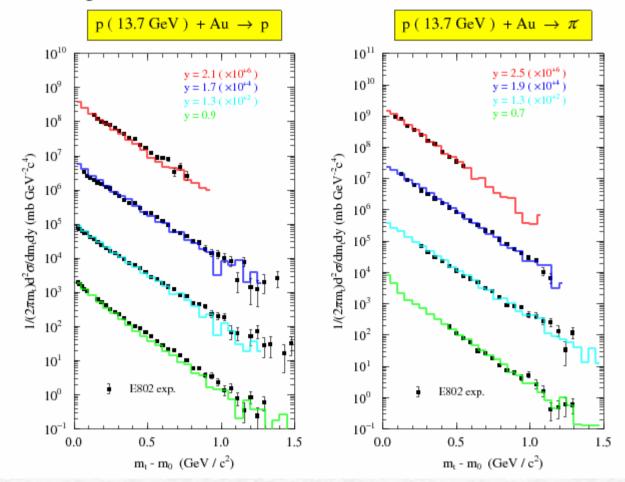
#### Other Hadron-Hadron Cross Sections

Parameterization of the total and elastic  $\pi$ -p and  $K^+p$  cross sections (upper panel), and the energy dependence of the exclusive cross sections of  $K^-p \rightarrow \pi^0 \Lambda$  and  $K^-n \rightarrow \pi^-\Sigma^0$  (lower panel).



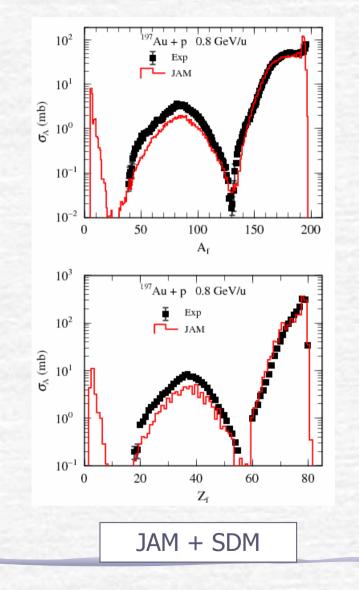
#### DDX of Nucleons and Pions from p-A Reactions

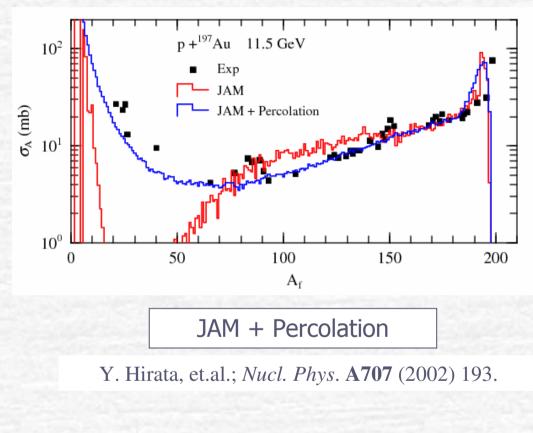
Invariant transverse mass distribution of proton (left panel) and  $\pi^-$  (right panel) from proton on thin Au target reaction at 13.7 GeV.



- 1. Two-body collision
- 2. Potential
  - 1). Initial ground state of target
    - Woods-Saxon for coordinates
    - Local Thomas-Fermi for momentum
  - 2). Frozen until participated
  - 3). Fixed square-well potential
  - 4). no reflection, no refraction

#### **Fragment Mass Distribution**



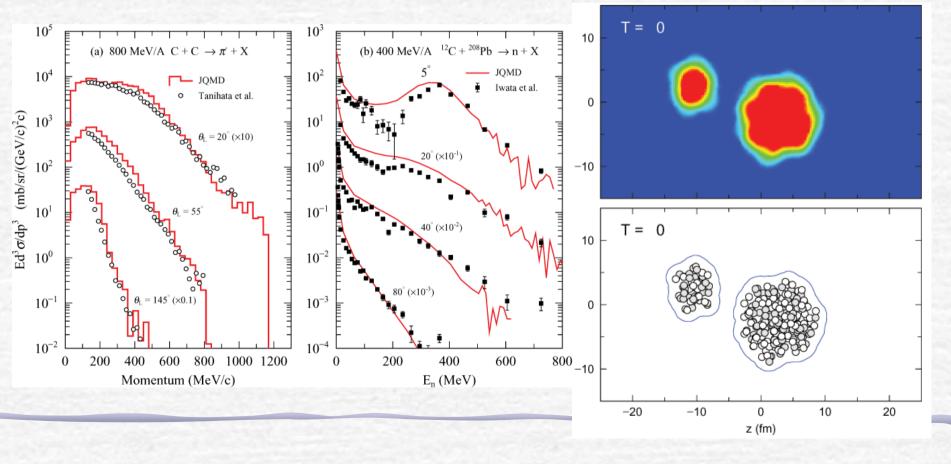


# JQMD code for Nucleus-Nucleus Collisions up to 100 GeV/u

JQMD (Jaeri Quantum Molecular Dynamics) for Simulation of Nucleus-Nucleus Collisions K. Niiita et.al. Phys. Rev. C52 (1995) 2620 http://hadron31.tokai.jaeri.go.jp/jqmd/

Analysis of Nucleus-Nucleus Collisions by **JQMD** 

<sup>56</sup>Fe 800 MeV/u on <sup>208</sup>Pb



# Basic Equations of QMD

Nucleon state (i) is represented by a Gaussian wave packet.

$$\phi_i(\mathbf{r}) = \frac{1}{(2\pi \mathbf{L})^{3/4}} \exp\left[-\frac{(\mathbf{r}-\mathbf{R}_i)^2}{4\mathbf{L}} + \frac{i}{\hbar} \mathbf{r} \cdot \mathbf{P}_i\right].$$

The one-body distribution function is obtained by the Wigner transform of the wave function,

$$f_i(\boldsymbol{r},\boldsymbol{p}) = 8 \cdot \exp\left[-\frac{(\boldsymbol{r}-\boldsymbol{R}_i)^2}{2L} - \frac{2L(\boldsymbol{p}-\boldsymbol{P}_i)^2}{\hbar^2}\right].$$

The equation of motion of  $R_i$  and  $P_i$  is given by the time-dependent variational principle,

$$\dot{\mathbf{R}}_i = \frac{\partial H}{\partial \mathbf{P}_i}, \quad \dot{\mathbf{P}}_i = -\frac{\partial H}{\partial \mathbf{R}_i}.$$

Hamiltonian H is given by

$$\begin{split} H &= \sum_{i} (m_{i}^{2} + P_{i}^{2})^{1/2} &: \text{Relativistic Energy} \\ &+ \frac{1}{2} \frac{A}{\rho_{0}} \sum_{i} \langle \rho_{i} \rangle + \frac{1}{1 + \tau} \frac{B}{\rho_{0}^{\tau}} \sum_{i} \langle \rho_{i} \rangle^{\tau} &: \text{Skyrme Terms} \\ &+ \frac{1}{2} \sum_{i,j(\neq i)} \frac{e_{i}e_{j}}{|R_{i} - R_{j}|} \operatorname{erf}(|R_{i} - R_{j}| / \sqrt{4L}) &: \text{Coulomb Potential} \\ &+ \frac{C_{s}}{2\rho_{0}} \sum_{i,j(\neq i)} c_{i}c_{j} \rho_{ij}, \quad c_{i} = \begin{cases} 1 \text{ for proton} \\ -1 \text{ for neutron} \end{cases} : \text{Symmetry Term} \end{split}$$

The density is given by  $\rho_i(\mathbf{r}) \equiv \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_i(\mathbf{r},\mathbf{p})$  $=\frac{1}{(2\pi L)^{3/2}}\exp\left[-\frac{(r-R_i)^2}{2L}\right].$ The overlap function is defined by  $\langle \rho_i \rangle \equiv \sum_{j \neq i} \rho_{ij} \equiv \sum_{j \neq i} \int d\mathbf{r} \ \rho_i(\mathbf{r}) \ \rho_j(\mathbf{r})$  $= \sum_{j \neq i} \frac{1}{(4\pi L)^{3/2}} \exp\left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{4L}\right].$ 

> The saturation condition of nuclear matter ( $\rho_0 = 0.168 \text{ fm}^{-3}, E_b = 16 \text{ MeV}$ )

$$A = -219.4 \text{ MeV}$$
  
 $B = 165.3 \text{ MeV}$ 

compressibility (K = 237.3 MeV)  $\tau = 4/3$ 

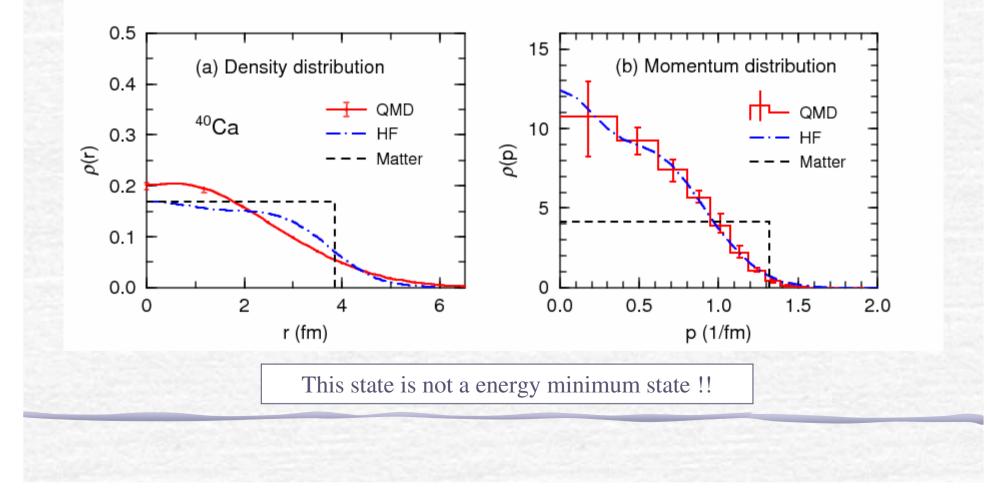
symmetry energy  $C_s = 25 \text{ MeV}$ 

Term

width of Gaussian (free parameter)  $L = 2 \, \text{fm}^2$ 

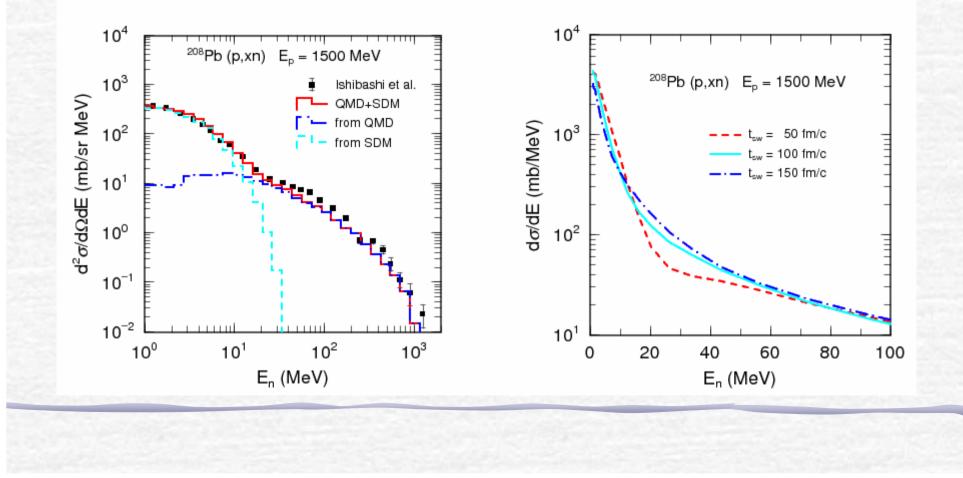
## Ground State of QMD

The ground state is generated by packing  $R_i$  and  $P_i$  randomly based on the Woods-Saxon distribution in the coordinate space and local Thomas-Fermi approximation in the momentum space. The ground state is a self-bind system and stable up to the time 200 fm/c.



## QMD + SDM (Statistical Decay Model)

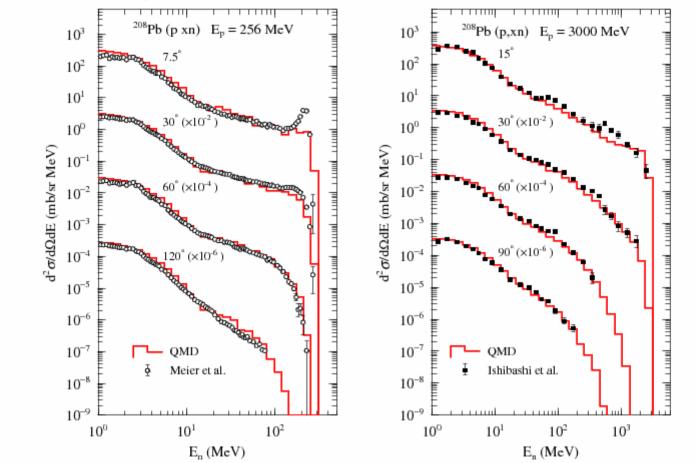
At the end of the dynamical stage, the QMD simulation yields many nucleons and fragments which are normally in highly excited states. We stop the QMD calculation and switch to the statistical decay model (SDM) at the end of the dynamical stage. The final results are not sensitive to the switching time if we use the switching time from 100 fm/c to 150 fm/c.



# **Nucleon Induced Reactions**

Neutron energy spectra for the reaction  $p + {}^{208}Pb$ . The incident energy is 256 MeV (left-hand-side) and 3 GeV (right-hand side). The solid histograms are the results of QMD and the open circles and the full boxes with error bars denote the experimental data.

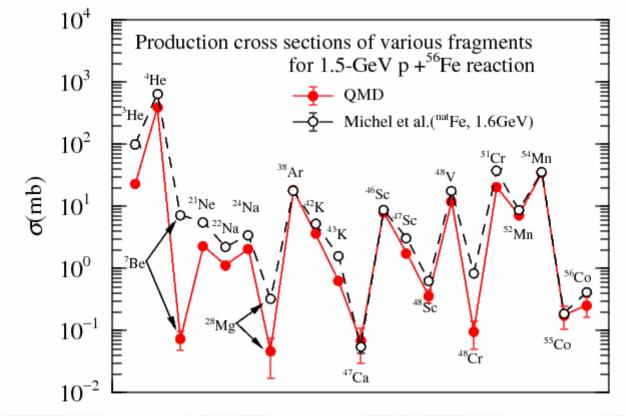
K. Niiita et.al. *Phys. Rev.* C52 (1995) 2620



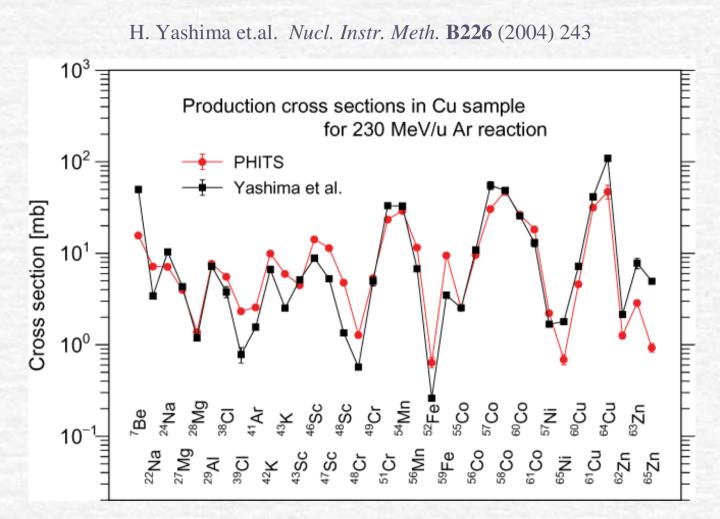
### **Nucleon Induced Reactions**

Production cross sections of various fragments for p  $(1.5 \text{ GeV}) + {}^{56}\text{Fe}$  reaction. The full circles connected by a solid line denote the results of QMD, while the open circles connected by a dashed line are obtained experimentally by Michel et al. measured at 1.6 GeV for  ${}^{nat}\text{Fe}$ .

S. Chiba et.al. Phys. Rev. C54 (1996) 285

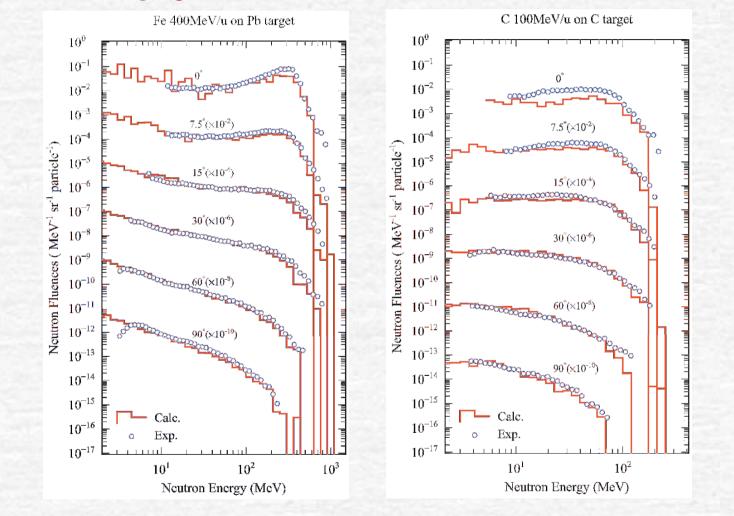






# Neutron Spectra from Thick Target

Introducing JQMD in PHITS : H. Iwase et.al. J. Nucl. Sci. Technol. 39 (2002) 1142

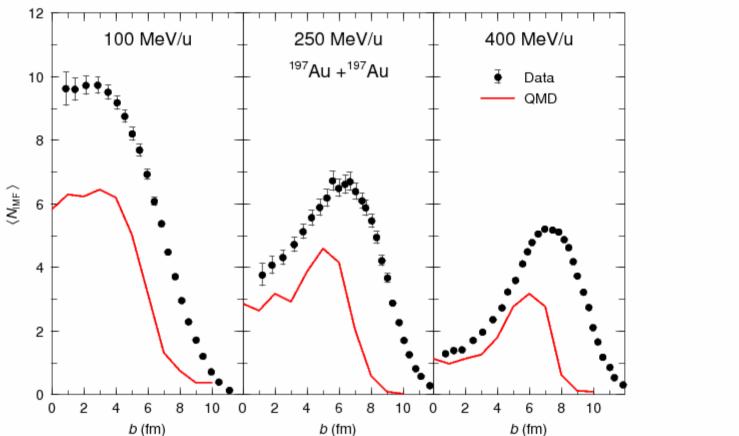


### Heavy Ion Reactions

**IMF** multiplicities for three incident energies (100, 250 and 400 MeV/nucleon) of Au + Au reactions as a function of the impact parameter b. The solid lines denote the results of the QMD, while the solid circles with error bars are the experimental data.

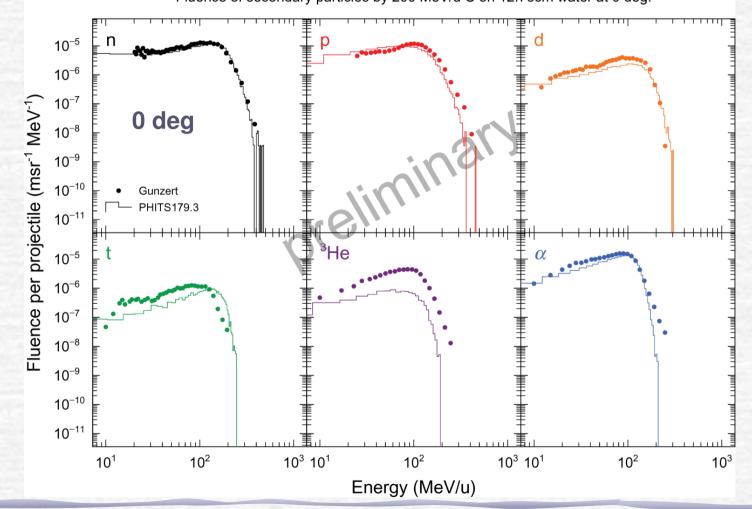
IMF  $3 \le Z \le 30$ 

T. Maruyama et.al. *Prog. Theor. Phys.* **98** (1997) 87

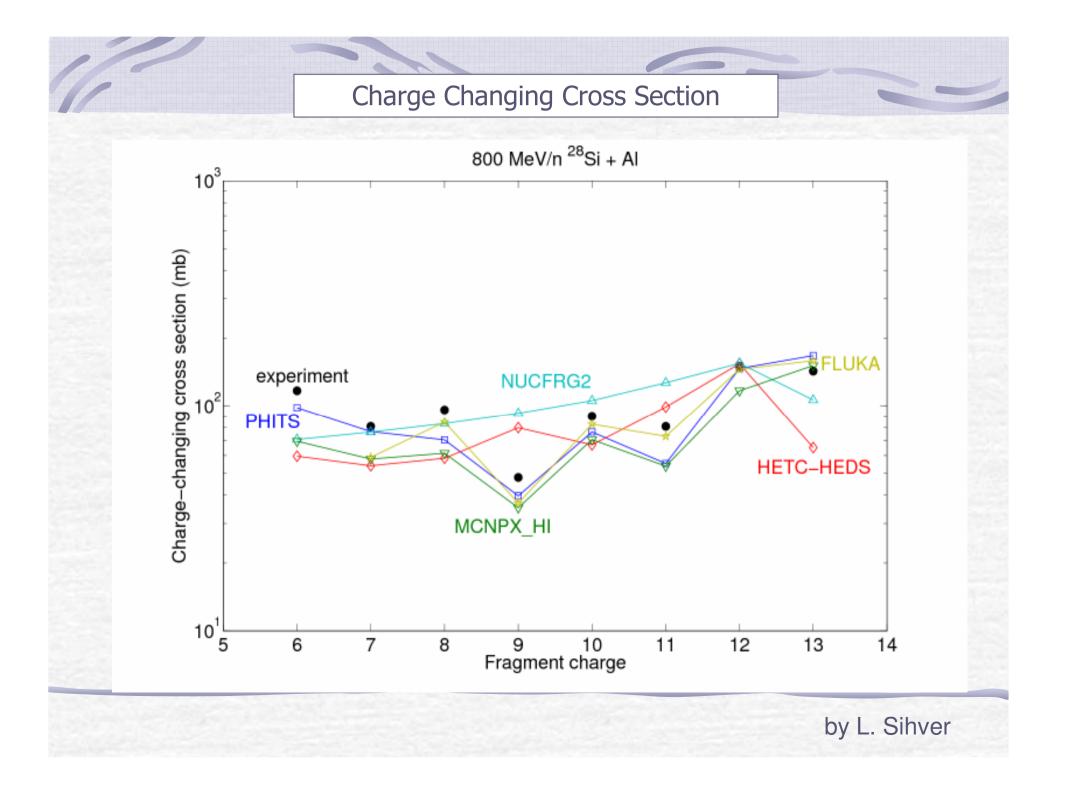


# Secondary Particle Production Cross Sections

#### From 200 MeV/u Carbon beam on 12.78 cm depth Water by K. Gunzert-Marx at GSI

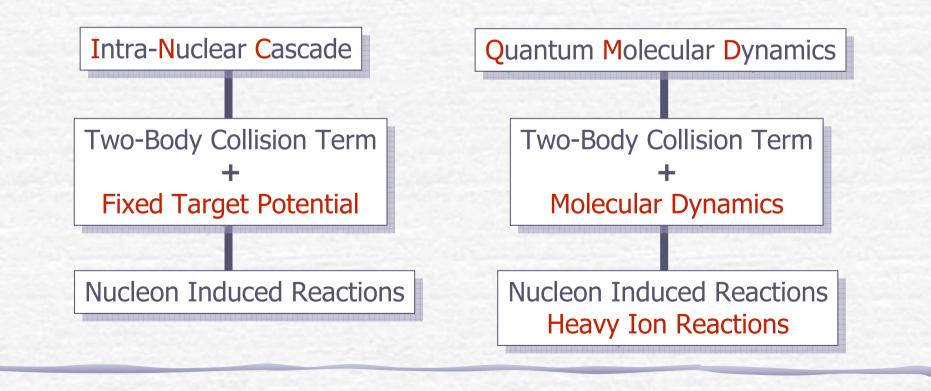


Fluence of secondary particles by 200 MeV/u C on 12.78cm water at 0 deg.



# Numerical Simulation for high energy nuclear reactions

- 1. Tow-Body Collision (hard interaction)
  - elementary cross sections for hadrons
- 2. Potential (soft interaction)
  - ground state, residual nucleus, excitation energy, recoil energy



Limitations and Problems both in JAM and JQMD

# 1. Tow-Body Collision term

- classical description : low energy limit independent sequential hadron-hadron collision de Broglie wave length « collision distances
- in-medium effects on elementally cross sections: free h-h cross sections are used for high energy, in-medium n-n cross sections are used for low energy How good ? It is related to the final Pauli blocking factor.
- Pauli blocking factor :

rigid Fermi sphere is assumed in JAM too rigid ? estimated from one-body phase space factor in JQMD huge fluctuation ?

 $\rightarrow$  FMD, AMD

Limitations and Problems both in JAM and JQMD

# 2. Potential term

• ground state :  $\rightarrow$  FMD, AMD

Momentum distribution : Local Thomas Fermi, no shell effect, no momentum dependent force

residual nuclei :

 (N,Z) and excitation energy,
 no information for collective motion nor deformation

 $\rightarrow$  connection to statistical decay models

# Limitations and Problems in JAM

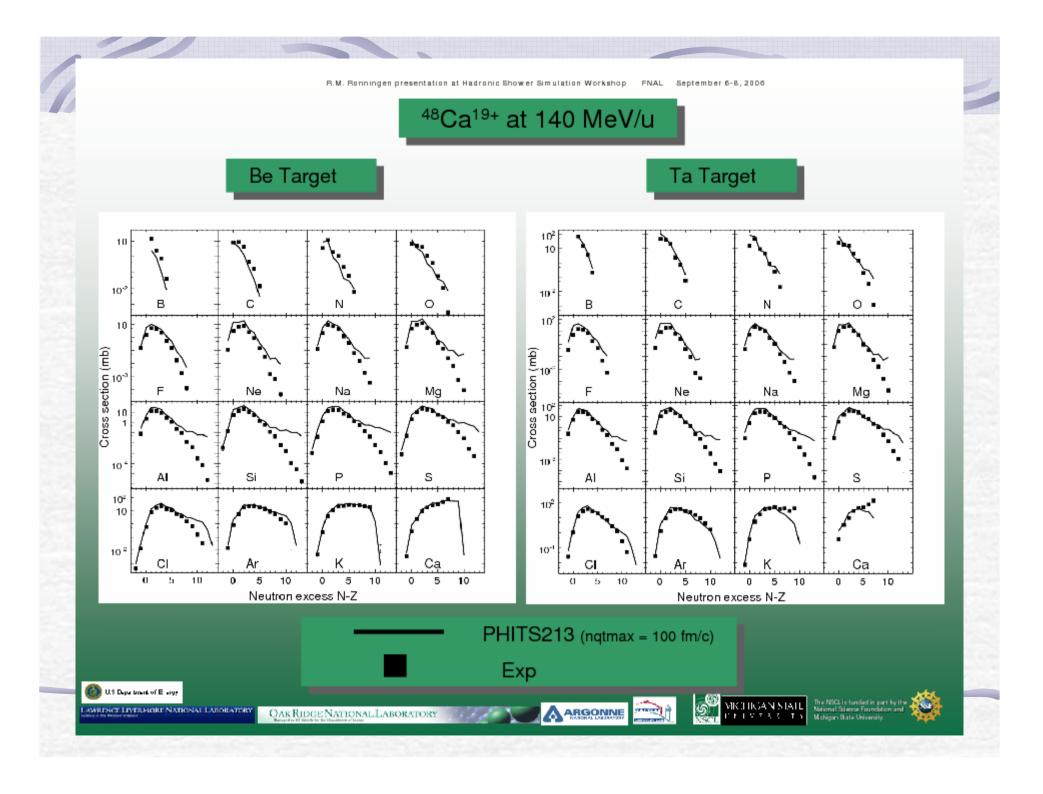
 Fixed target potential : no dynamical change of nucleus, no cluster emission in the dynamical stage

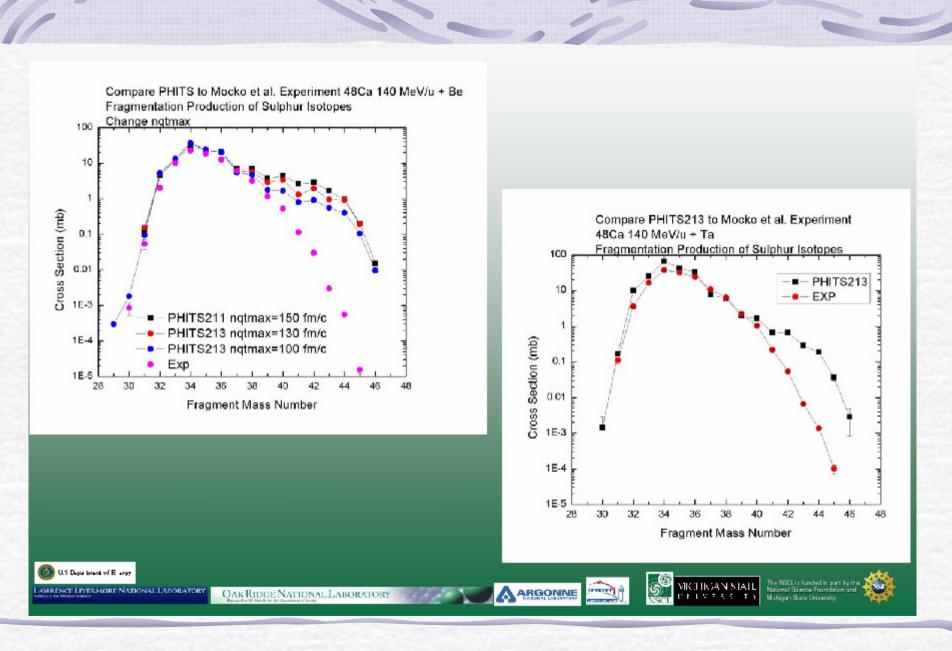
Limitations and Problems in JQMD

• Nucleus : described as a self-binding system dynamical change of nucleus, cluster emission ??

- ground state is not a energy minimum state
   → spontaneous emission of nucleons
- not fully relativistically covariant
  - $\rightarrow$  unstability of nucleus after boosting
- connection time to statistical model
   → over cooling of the residual nucleus

Solved by new R-JQMD (Relativistic JQMD) by D. Mancusi





Strategy for better description of nuclear reactions

In PHITS,

Dynamical models (JAM, JQMD) + Statistical Decay model (GEM) can well describe the energetic secondary particles, particularly, neutrons, which are very important for the transport phenomena in material.

However, some cross sections of the fragments are not good.

- $\rightarrow$  add more sophisticated effective interactions
- $\rightarrow$  AMD, FMD
- $\rightarrow$  add new models
  - pre-equilibrium model,
  - Fermi breakup, percolation, ....

**Strategy** for better description of nuclear reactions

Our strategy for this : If you need only one-body inclusive quantities, we use evaluated nuclear data for the fragment cross sections or some other cross sections.

For an example, for the activation of air and water, we can use the following cross section data for the yield tally in PHITS.

$^{4}$ He(n,x) $^{3}$ H	$^{14}N(n,x)^{3}H$	${}^{14}N(n,x)^{7}Be$	$^{14}N(n,x)^{11}Be$	$^{14}N(n,x)^{10}C$	$^{14}N(n,x)^{11}C$
$^{14}N(n,x)^{14}C$	$^{14}N(n,x)^{13}N$	${}^{16}O(n,x)^{3}H$	${}^{16}O(n,x)^7Be$	$^{16}O(n,x)^{11}Be$	${}^{16}O(n,x){}^{10}C$
${}^{16}O(n,x){}^{11}C$	$^{16}O(n,x)^{14}C$	<sup>16</sup> O(n,x) <sup>15</sup> C	${}^{16}O(n,x){}^{13}N$	<sup>16</sup> O(n,x) <sup>16</sup> N	<sup>16</sup> O(n,x) <sup>14</sup> O
$^{16}O(n,x)^{15}O$	<sup>4</sup> He(p,x) <sup>3</sup> H	$^{14}N(p,x)^7Be$	<sup>14</sup> N(p,x) <sup>11</sup> Be	$^{14}N(p,x)^{10}C$	$^{14}N(p,x)^{11}C$
$^{14}N(p,x)^{13}N$	$^{14}N(p,x)^{14}O$	<sup>16</sup> O(p,x) <sup>3</sup> H	<sup>16</sup> O(p,x) <sup>7</sup> Be	<sup>16</sup> O(p,x) <sup>11</sup> Be	${}^{16}O(p,x){}^{10}C$
${}^{16}O(p,x){}^{11}C$	${}^{16}O(p,x){}^{14}C$	${}^{16}O(p,x){}^{13}N$	${}^{16}O(p,x){}^{14}O$	<sup>16</sup> O(p,x) <sup>15</sup> O	