Towards modularization and vectorization of Geant4 physics: a pilot study

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SLAC-FNAL Pilot Project on Geant R&D funded by DOE

Explore new computing avenues for HEP simulation

- Sharable and modularized components
- Modern hardware technologies and parallel architectures
- Key R&D needs and cross-cutting solutions

Inter-US-national-laboratory collaboration

- Modularize Geant4 Bertini cascade model and first pass algorithm optimization – SLAC (T. Koi)
- Vectorized a sub-part of the model – G. Lima (FNAL)
- Integrate and evaluate performance gains – FNAL (S.Y. Jun)
- Identify requirements for future extension/development

A pilot project for developing a common hadronic simulation model for Geant4 and GeantV

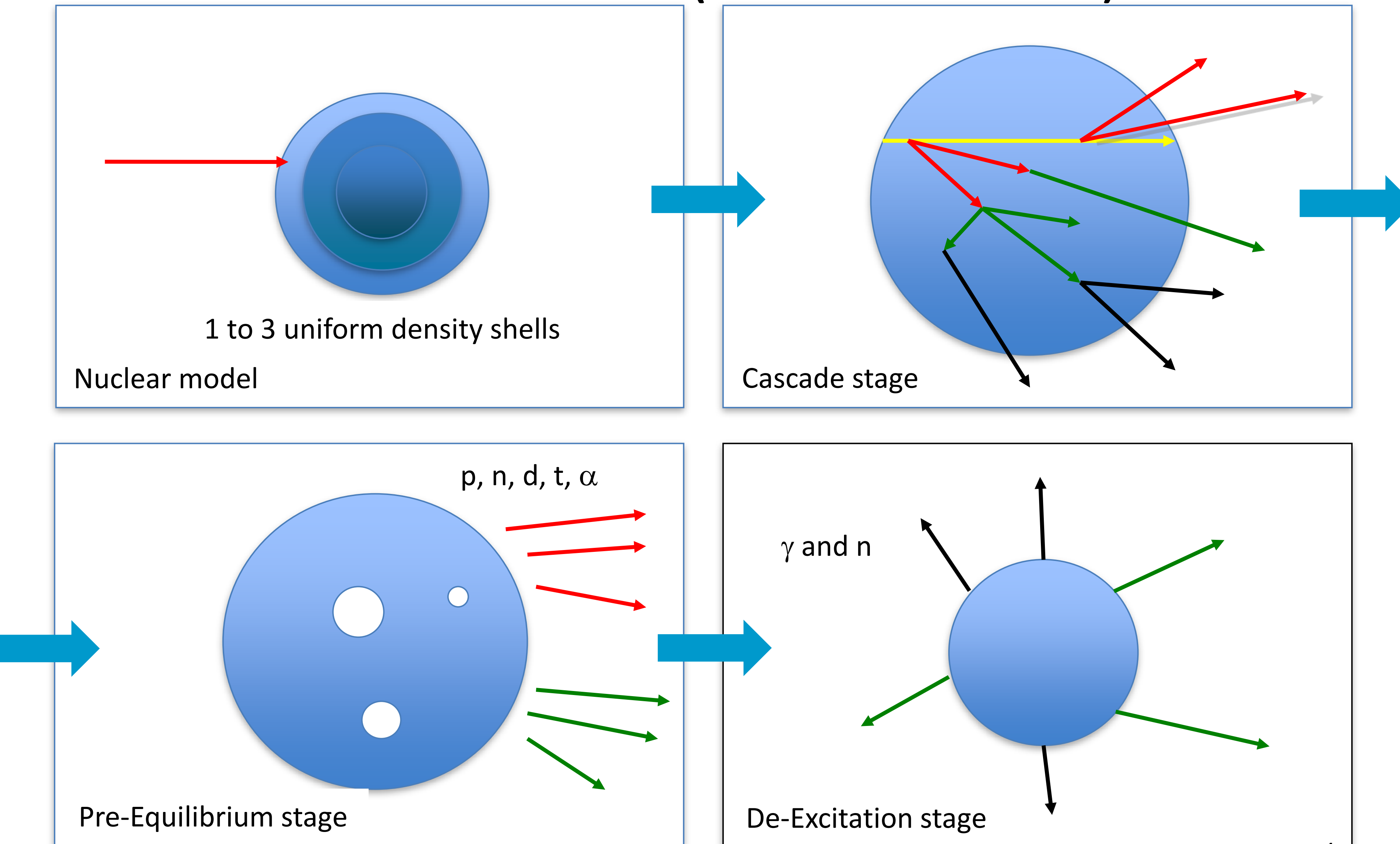
Accurate modeling of the 0~12 GeV energy range for hadrons is crucial for achieving good simulated response in calorimeters and thick targets.

The Geant4 Bertini-style (BERT) cascade is the preferred model for hadron-nucleus interactions in this region.

- It handles the large range of energies and particle types
- relatively fast calculation speed than other cascade models (Binary and INCL) of Geant4
- The pre-equilibrium and de-excitation phases of the nuclear interaction are already contained within the model.

Therefore, the BERT Model is selected for the target model of the pilot project.

Schematic view of BERT Cascade (0 < E < 15GeV)



Geant4 Bertini Cascade Model in Geant4

A classical (non-quantum mechanical) cascade

- Simple shells structure of target nuclear model
- Average solution of a particle traveling through a medium (Boltzmann equation)

Core code:

- Elementary particle collisions with individual protons and neutrons:
  - free space cross sections used to generate secondaries
- Cascade in nuclear medium
- Coalescence models for emission of light nuclei from cascade stage
- Pre-equilibrium and equilibrium decay of residual nucleus

In Geant4 the Bertini cascade is used for p, n, π^+, π^-, K^+, K^-, K^0_L , K^0_S, Λ , Σ^0 , Σ^+ , Σ^- , Ξ^0 , Ξ^-, Ω^- and γ

- Valid for incident energies of 0 – 15 GeV

GXBERT:
Modularized version of BERT Cascade Model of Geant4

At the first step of the project, we made a standalone version of Geant4 BERT Model.

- Remove all dependency to Geant4 (G4Material, G4Track/Step objects, etc) from the model.

This modularization was done under conditions of

- Allow dependency to CLHEP library.
- Keep physics capability of BERT as much as possible.
  - However, turned off “optional” interfaces to utilize Geant4 pre-compound and de-excitation models.
- Ignore the special treatments in the model for multithreading applications.

GXBERT can run as a backend of Geant4 and also standalone application

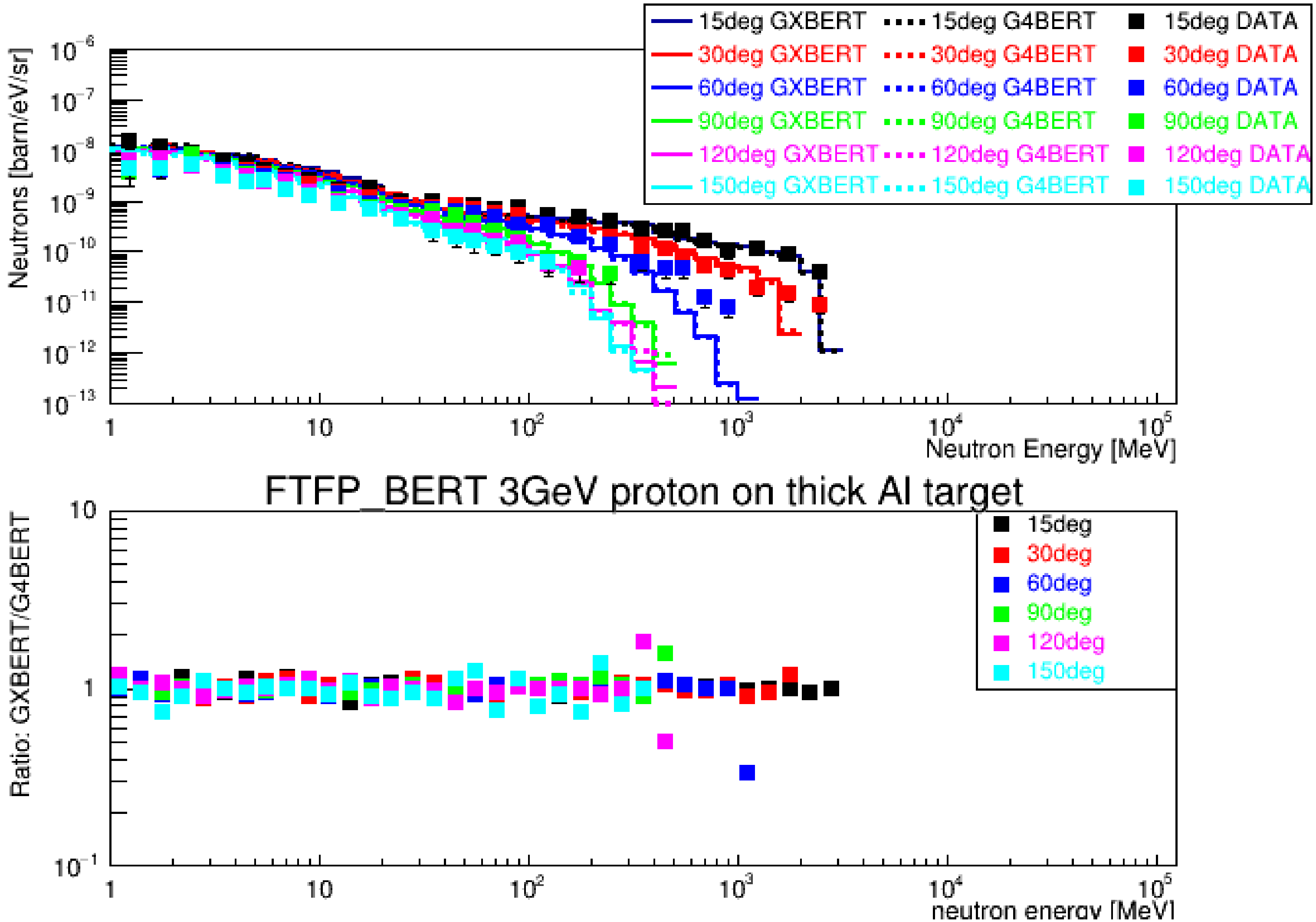
1, Using GXBERT in a Geant4 application

- GXBERT acts like a hadronic model of Geant4
- The application includes “geometry”, “physics list” and many other Geant4 components for full detector simulation

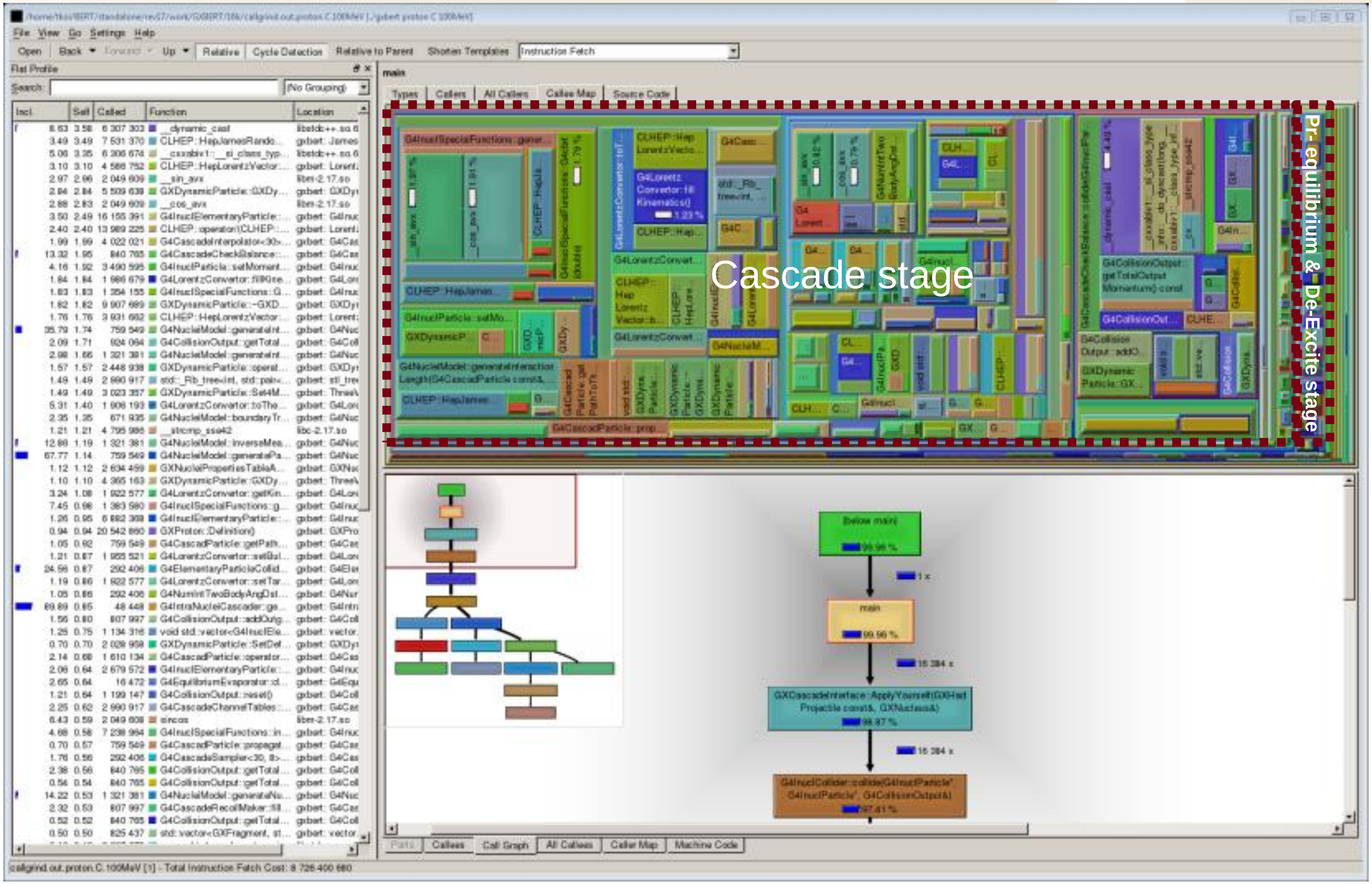
2, Using GXBERT in an application without Geant4 library

- GXBERT acts as a reaction model
- Physics and computing performances are compared to equivalent Geant4 application

Preliminary Physics Validation of GXBERT



Optimization of GXBERT



Optimization of GXBERT

Confirmed previous conclusions (based on full applications): for detector simulations there are no single kernel with important fractions of CPU

Three components for CPU (each several kernels)

- Cascade stage spends 90% of CPU time
  - This stage includes coalescence sub-model
- Pre-Equilibrium and De-Excitation stage spends10% of CPU time
- Clustering calculation in the coalescence sub-model spends non negligible amount of CPU time in high energy and high Z target interactions

Optimization of GXBERT

Although there is no major bottle neck, based on code review and profiling result, followings parts are optimized

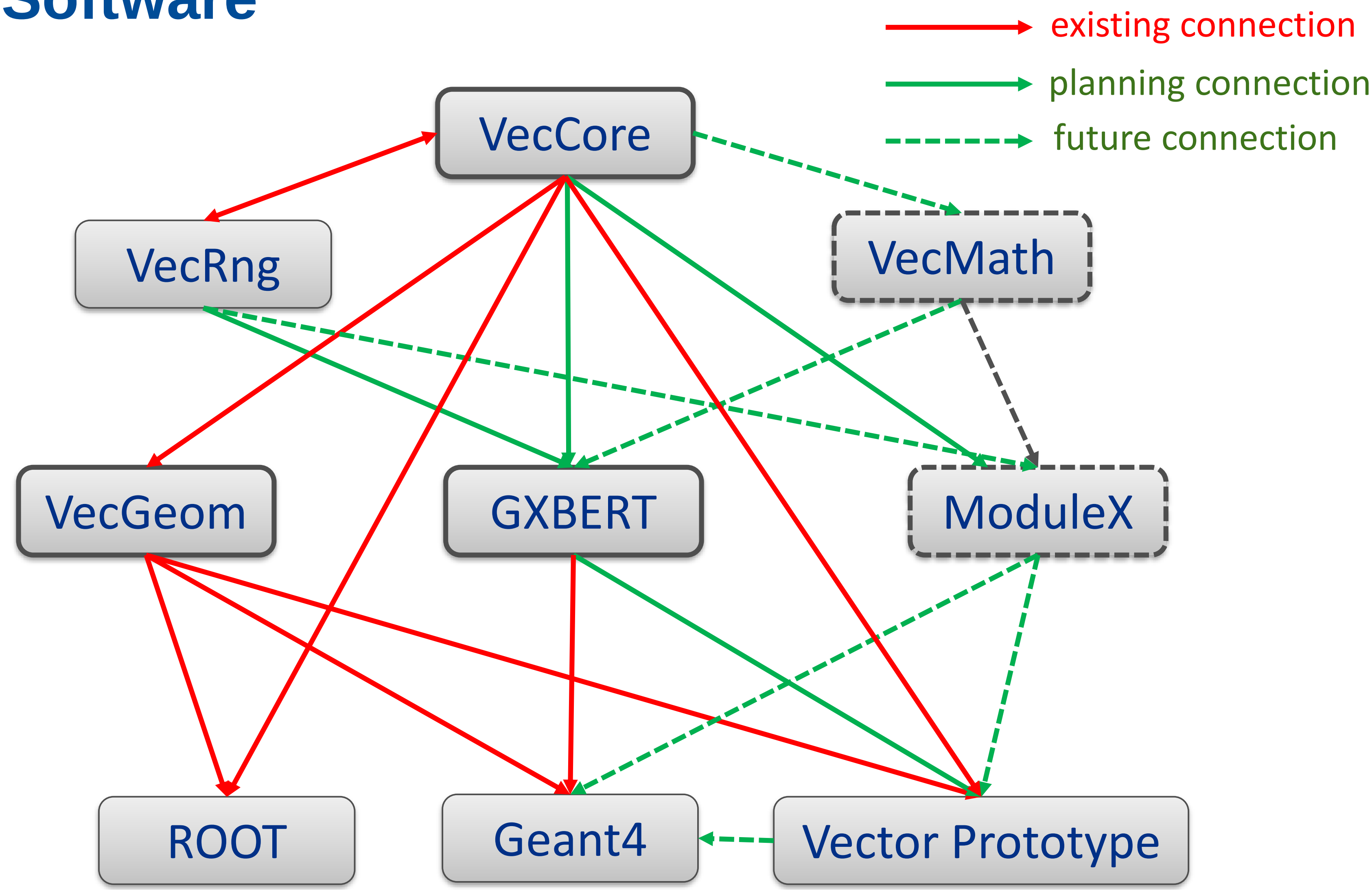
- “cbrt” function
- member of “DynamicParticle”
- constructor and destructor of “DynamicParticle”
- “InuclElemntaryParticle::type()” method
- Implementation of singleton classes of “Proton” and “Neutron”

After these optimizations, total performance of GXBERT is improved of 13-25% with respect to Geant4-Bertini

Vectorization

- Support both sequential (scalar) and parallel (vector) particle transport with a common code
  - VecCore: hide architectures (SIMD instruction sets and GPU)
  - Simplify layers of workflows and decompose tasks as units of vector(parallel) tasks
  - Add multiple particles or vector interfaces (tracks, vector-type of input, SOA, etc.)
- Minimal dependencies
  - Identify external common components for vectorization (à la vector version of CLHEP)
    - Parallel random number generation (VecRng) – ready to use
    - Math library (VecMath) – add a minimal set for HEP
    - Data structure (container classes) for vectorization

Vectorization of GXBERT and Relationship to Other HEP Software



Summary

A pilot project to kick-start physics-level modularization was launched with three goals:

- Study feasibility of removing dependency from G4 at the physics model level: DONE (SLAC)
- First pass optimization (code reviews). 13-25% speedup achieved: DONE (SLAC)
- Preliminary computing performance evaluation: Done (FNAL)
- Original Bertini code was already fairly optimized
- Vectorization of a sub-part of the Bertini model: TO BE DONE (FNAL)

GXBERT is a standalone hadronic model

- Provided as a open-source code on gitlab as a starting point for further studies

Back up slides

History of BERT Cascade Model of Geant4

~2002 – adaptations of Bertini (INUCL) to the Geant4 hadronic framework

2003 – add kaon production and interaction

2004 – add hyperon production and interaction

2007 – add “optional” interfaces for other pre-compound and evaporation models in Geant4

2008-2010 – code optimized for memory consumption and speed

2011 – add coalescence models for emission of light nuclei

2012 – migration to multithreading library

2013 – add gamma nuclear interactions

2015-2018 – ongoing extensions to 9-body final states for hadron-nucleon reactions

Dependencies of BERT Cascade Model of Geant4

Dependencies on Geant4

Global

- IO related
  - G4cout,,,
- Type
  - G4double,,,
- Multithreading
  - G4Threading, G4AutoLock,,,
- Allocator
- State related
- Exception handling

Particle

- G4Proton,,,
- G4ParticleTable, G4IonTable
- Ion mass table

Hadronic framework

- G4HadronicInteraction,,,

Decay

- Decay Channel, Decay Algorism,,,

,,,

Dependencies on CLHEP

Vector

- 4 and 3 vector
- Rotation

Random

- Random number generator

Remain as this
Port to GXBERT
Exclude from GXBERT