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Vectorization of Bertini cascade

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* T.Koi is not active in this project anymore

Outline

- Introduction
  - motivations, goals and scope
- Progress
  - process flow and vectorization
  - features request
  - preliminary results
- Current status and prospects

SLAC-FNAL pilot project on Geant R&D

Explore new computing avenues for hadronic physics simulation in HEP

Hadronic simulation is an important missing component of the GeantV transport engine. It is the *next logical step* beyond EMphys vectorization (regular number and types of secondaries), with variable numbers of secondaries and simulation steps in each interaction.

Bertini cascade was chosen for this project, since it is the preferred model for low energy hadron-nucleus interactions and it handles a large number of particle types.

Goals

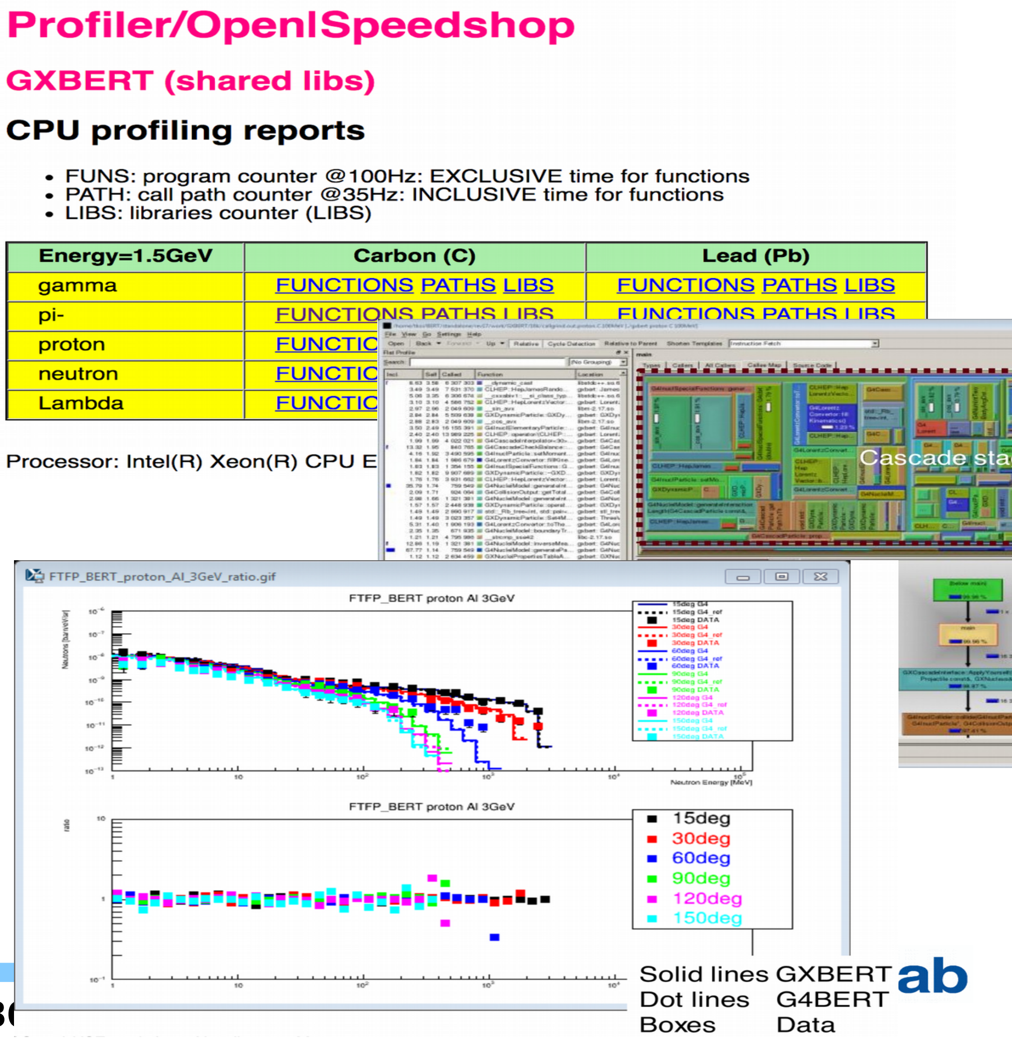
- Provide standalone, vectorized Bertini algorithms (a specific hadronic cascade model)
- Modularized components, compatible with both Geant4 and GeantV transport (like VecGeom)
- Efficient utilization of modern hardware technologies and parallel architectures

Project scope

- Modularize Geant4 Bertini cascade model and optimization – T.Koi (SLAC)
- SIMD vectorization of some computing-intensive algorithms – G. Lima (FNAL)
- Integration and computing performance evaluation – S.Y. Jun (FNAL)
- Identify requirements for future extensions and development

Implementation details and choices

- Use detailed profiling to identify some CPU-heavy algorithms to demonstrate performance gains from vectorization
- Redesign data structures to promote vectorization with minimal overhead (*SoA structures*)
- Use templated types to write generic kernels to be instantiated using scalar or vector types as needed
- VecCore package to isolate complexities of vectorization implementation from algorithm kernels
- Benchmark every vectorized class, for close performance monitoring
- Validate physics simulation results with respect to Geant4



Progress on Bertini vectorization

- Combining a top-down approach…
  - **Vectorizing function interfaces (passing SIMD-vectors down into algorithms)**
  - Vectorized utilities (e.g. rotations, Lorentz boosts, …) and data structures (InuclParticle and InuclElementaryParticle classes)
  - Processing flow: lots of sanity checks and triage based on particle types

    → assume homogeneous SIMD-vector inputs – e.g. [p][C] becomes [pp…p] onto [CC…C]

    → hadron-hadron, hadron-nucleus, nucleus-nucleus collisions (algorithm functions → vectorized kernels)

- … and a bottom-up approach
  - Follow processing flow all the way to the innermost (leaf) algorithms
  - Generic kernels for generating multiplicity, particle types, kinematics (momenta, angles)
    - hadron-hadron collisions: class G4ElementaryParticleCollider (lots of non-trivial functions)
  - Math functions – Log, Exp, Pow, Factorial, LogFactorial – have fast implementations for integer arguments
  - Currently vectorizing the functions to generate multiplicities and final states (PIDs and kinematics), and their validation tests and benchmarks

- Next pages, pseudo-code is used to illustrate vectorization progress, and rationale behind suggestions for algorithmical changes

Class G4ElementaryParticleCollider

Functions: generateSCMfinalState( ), generateMultiplicity( ), generateOutgoingPartTypes( )

```
** class G4ElementaryParticleCollider : public G4CascadeColliderBase : public G4VCascadeCollider
*** Constructor: trivial
*** G4ElementaryParticleCollider::collide(bullet, target, output)...
*** G4ElementaryParticleCollider::generateSCMfinalState(ekin, etot_scm, particle1, particle2)
+ loop to generate valid final state (itry_max = 10)
  + clear output vectors
  + multipl = generateMultiplicity(initState, ekin)          <=== [vectorized]
  + generateOutgoingPartTypes(initState, multipl, ekin)      <=== [vectorizable (imultipl?)]
  + fillOutgoingMasses()   // cache each particle mass, mass2      [vectorized (imultipl?)]
    // Attempt to produce final state kinematics
  + fsGenerator.Configure(particle1, particle2, particle_kinds);    <=== [being vectorized (imultipl?)
  + generate = !fsGenerator.Generate(etot_scm, masses, scm_momentums);  <=== [being vectorized]

+ if any problems, return (no valid final state)
+ store final state particles (and their SCM kinematics)
+ return

*** G4ElementaryParticleCollider::generateMultiplicity(initState, ekin)
+ xsecTable = G4CascadeChannelTables::GetTable(initState);
+ if (xsecTable) multipl = xsecTable->getMultiplicity(ekin);
+ return multipl;

*** G4ElementaryParticleCollider::generateOutgoingPartTypes(initState, multipl, ekin)
+ particle_kinds.clear()        // Initialize buffer for generation
+ xsecTable = G4CascadeChannelTables::GetTable(initState)
+ xsecTable->getOutgoingParticleTypes(particle_kinds, mult, ekin)
+ return particle_kinds
```

Are these possible to be vectorized? *Maybe*, if and only if multiplicity is homogeneous

Experiment with intra-algorithm re-basketization

See backup slides for more details on this processing flow!

G4CascadeFinalStateAlgorithm class

```
** class GXCascadeFinalStateAlgorithm : public GXVHadDecayAlgorithm
*** GXCascadeFinalStateAlgorithm::Configure(bullet, target, particle_kinds)
{
  // Identify initial and final state (if two-body) for algorithm selection
  multiplicity = particle_kinds.size();        <=== must be same multiplicity
  G4int is = bullet->type() * target->type();
  G4int fs = (multiplicity==2) ? particle_kinds[0]*particle_kinds[1] : 0;

  ChooseGenerators(is, fs);    <=== probably vectorizable IFF particle_kinds[2] is homogeneous

  // Save kinematics for use with distributions
  SaveKinematics(bullet, target);      <=== [vectorized]

  // Save particle types for use with distributions
  kinds = particle_kinds;
}

*** GXCascadeFinalStateAlgorithm::ChooseGenerators(bullet, target, particle_kinds)
{
  // Choose generator for momentum
  if (G4CascadeParameters::usePhaseSpace()) momDist = 0;
  else momDist = G4MultiBodyMomentumDist::GetDist(is, multiplicity);

  // Choose generator for angle
  if (fs > 0 && multiplicity == 2) {
    G4int kw = (fs==is) ? 1 : 2;
    angDist = G4TwoBodyAngularDist::GetDist(is, fs, kw);
  } else if (multiplicity == 3) {
    angDist = G4TwoBodyAngularDist::GetDist(is);
  } else {
    angDist = 0;
  }
}
```

Several different objects returned depending on
is (initial state),
fs (final state)
and multiplicity

Redesigning for vectorization

- Keep SIMD lanes synchronized for best vectorization performance
  - GeantV basketizer: homogeneous baskets of particles in given detector volumes (geometry + materials)
  - Avoid/minimize divergence between SIMD lanes: branches into distinct blocks of code (even algorithms/models)

- Hadronic processes tend to diverge quickly
  - GeantV baskets: homogeneous input arrays for simulation
    - e.g. [pp...p] on [Scint, Scint, ... Scint]
    - Bertini case: protons will collide with either C-atoms or H-atoms

    → rebasketizing here will promote higher levels of lane synchronization
  - from previous slide: multiplicity-based basketization is particularly important for Bertini algorithms
    - both final state and kinematics sampling algorithms are based on multiplicity

    → rebasketizing by multiplicity promotes the development of more efficient Bertini kernels (→ max synchronization)

  → planning to use track re-basketization based on multiplicity, and maybe final state too

- Another challenge: dealing with Vector<int> and Vector<double> in the same algorithms
  - VcVector<long int> is not supported by Vc library
  - Work-around (a bit too technical!): using Int_v = VcSimdArray<VectorSize<Real_v>> to create SIMDVectors of *ints* corresponding to *doubles*

  → best long-term solution: native suport from VecCore (under discussion with VecCore developers)

Two illustrative preliminary results

- Unit test for InuclElementaryParticle

```
lima@mac: build  ./TestInuclElementaryParticle
=== GXInuclElemParticles:  Particles=[proton; neutron; gamma; deuteron] masses=[938.272; 939.565; 0; 1875.61] types=<1 2 9 41> ekin=[1073.52, 925.289, 827.232
, 1155.82]
4 tracks: <1 2 9 41>
 kinE=[1073.52, 925.289, 827.232, 1155.82]
 totE=[1073.52, 925.289, 827.232, 1155.82]
 nucleon:m[1100]
 pion:m[0000]
 photon:m[0010]
 baryon:<1 1 0 2>
 strange:<0 0 0 0>
 quasi_deutron(): m[0000]
=== GXInuclElemParticles:  Particles=[pi+; pi-; diproton; dineutron] masses=[139.57; 139.57; 1876.54; 1879.13] types=<3 5 111 122> ekin=[1073.52, 925.289, 827
.232, 1155.82]
4 tracks: <3 5 111 122>
 kinE=[1073.52, 925.289, 827.232, 1155.82]
 totE=[1213.09, 1064.86, 2703.78, 3034.95]
 nucleon:m[0000]
 pion:m[1100]
 photon:m[0000]
 baryon:<0 0 2 2>
 strange:<0 0 0 0>
 quasi_deutron(): m[0011]
>>> GXInuclElementaryParticle tests passed.
```

New SoA data structures can handle particles of different types

- Benchmark for GXLorentzConvertor (~4x faster)

```
lima@mac: build  ./LorentzConvertorBenchmark 3.0 1048576 10
GXBert results:   sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 100.117
Scalar results:   sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 63.2348
Vector size: 4
Vector results:   sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 14.7479
VectorL result:   sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 14.6649


GXBert results:   sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 100.376
double results: sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 63.1925
Double_v results: sumEscm = 1.96957e+09   sumEkin = 3.75451e+06   sumP2 = 9.23118e+11   CPUtime = 14.451
```

Vectorizing math functions

- Bertini algorithms use some “fast math functions” available in Geant4
  - “fast”: pre-calculations cached for integer arguments
  - cached exp(x) for integer or half-integer x, truncated O(x^3) Taylor series for |x|<84 (fully vectorized), otherwise use VDT implementation (internal vectorization, also used by Geant4)
  - cached log(x) for integers up to 512, otherwise use VDT implementation
  - specialized Pow(x,y) for integer x or y, etc…

- Fully vectorized versions are hard to implement
  - e.g. Pow([x1, x2, x3, x4], [n1, n2, n3, n4])
  - vectorize interface only, [Pow(x1,n1), Pow(x2,n2), Pow(x3,n3), Pow(x4,n4)]
    - scalar functions are called once per lane, to build the SIMD vector
    - this is actually how it is done in VecCore, for commonly used math functions like Sin(), Cos(), Abs(), …
    - slower than original implementation due to SIMD storing overhead
  - the vectorized interface is useful to simplify vectorization of mathematical expressions involving such functions (maybe worthy the overhead)
  - some vectorization is possible on some of the “fast” versions

- See next pages for some performance comparisons

Benchmarking math functions

- Preliminary measurements of *relative performance* (AVX)
  - Original: Geant4 "fast" implementations for integer arguments (global/management)
  - Scalar, Vector: my "vectorized interface" versions, templated on scalar or vectorized types, calling Geant4 "fast" implementations
  - ScalarStd, VectorStd: same as above, but calling std::functions instead of the Geant4 "fast" implementations

```
* ./ExpABenchmark: exp(x)

ExpA() Benchmark: nReps=100 and nvals=2097152

 Original ExpA(): 3.53498e+227 1334.87 msec
   Scalar ExpA(): 3.53498e+227 1339.55 msec
   Vector ExpA(): 3.53498e+227 1365.73 msec
Scalar ExpAVec(): 3.53498e+227 1455.18 msec
Vector ExpAVec(): 3.53498e+227 626.344 msec
ScalarStd ExpA(): 3.53498e+227 1241.94 msec
VectorStd ExpA(): 3.53498e+227 1184.67 msec
```

Fully vectorized fast algo — ~2x

```
* ./LogZBenchmark: log(n)

LogZ() Benchmark: nReps=100 and nvals=2097152

 Original LogZ(): 8.73641e+06 239.454 msec
   Scalar LogZ(): 8.73641e+06 530.022 msec
   Vector LogZ(): 8.73641e+06 238.823 msec
ScalarStd LogZ(): 8.73641e+06 1096.34 msec
VectorStd LogZ(): 8.73641e+06 1183.11 msec
```

Int argument, cached — ~4x

```
* ./PowZBenchmark: Z^x

PowZ() Benchmark: nReps=100 and nvals=2097152

 Original PowZ(): 2.01829e+17 1335.01 msec
   Scalar PowZ(): 2.01829e+17 1692.68 msec
   Vector PowZ(): 2.01829e+17 1446.95 msec
ScalarStd PowZ(): 2.01835e+17 3893.61 msec
VectorStd PowZ(): 2.01835e+17 3844.93 msec
```

Integer base, cached — ~2x

- Preliminary conclusion: overhead of vectorized interface is significant, but it is probably worth the convenience
- There probably is room for performance improvements
- In some cases, the *fast* Geant4 implementation is not better than the standard version, so we can use it for those cases.

Current status

- What has been accomplished so far
  - Git repository available: https://github.com/gxbert/gxbert.git
  - Basic infrastructure for development, unit testing and performance evaluation (v01 done)
  - New SoA data structure for tracks and kinematics (v01 done, extensions needed for nuclei)
  - Vectorized ThreeVectors (~CLHEP interface) and LorentzVectors (done)
    - to become part of the VecMath library
  - Basic algorithms for Lorentz boosts (Lab frame ↔ projectile ↔ center of mass frame) as needed (done)
    - measured speedups of up to ~4x in avx mode (theoretical max = 4) w.r.t. scalar mode
    - additional 25% gain (scalar vs. G4), due to less branching and better memory locality
  - Integration of Soon's vectorized pRNG (pseudo-Random Number Generator) (done, not yet from VecMath)

Prospects

- What can be done in the short- to medium-term (h-h interactions only)?
  - Currently vectorizing algorithms that handle hadron-hadron interactions (under way)
  - Finalizing vectorized interfaces for all parts of processing flow (under way)
  - Vectorization of all algorithms which can deal with homogeneous input (under way)
  - Unit tests and benchmarks for vectorized functions (partly done = keeping up)
  - I am more optimistic now than at the beginning of this project.

- What requires more time
  - Full cascade algorithms – it is a long process, because of the large number of non-trivial functions involved.
    - [see backup slides for more details on the Bertini processing flow]
  - Supporting tools will be very helpful
    - Intra-algorithm re-basketization in GeantV
    - Native support to Vector<double> ← → Vector<int> in VecCore
  - Full vectorized prototype corresponding to Tatsumi's tests for hadron-nucleus toy experiments, showing some speedup due to vectorization (not started)
  - Vectorization of hadron-nucleus and nucleus-nucleus processes (is Bertini used for those?)
  - profiling-based optimization of vectorized algorithms
  - Full assessment of performance gains from vectorization → further performance optimization

Backup slides

Bertini processing flow

- Start from Tatsumi's example, gxbertTest, which:
  - Sets up a large number of homogeneous collisions (e.g. projectiles(=protons) on targets(=Lead)
  - calls GXCascadeInterface::ApplyYourself(bullet,target) for each pair

```
** class GXCascadeInterface
*** GXCascadeInterface::construtor()
*** GXCascadeInterface::ApplyYourself(GXHadProjectile, GXNucleus)
+ sanity checks
+ fill bullet params
  either hadronBullet:  G4InuclElementaryParticle    <=== [vectorized]
      or hadronNucleus: G4InuclNuclei
+ fill target params
  either targetBullet:  G4InuclElementaryParticle    <=== [vectorized]
      or targetNucleus: G4InuclNuclei

+ loop {
    collider->collide(bullet, target, output)      <=== [being vectorized] (more details below)
    balance->collide(bullet, target, output)
  } until( 20 iterations or final state valid )

+ rotate final state back to lab frame             <=== [vectorized]
+ convert result (final state) from
  Bertini format          to       GX format
  ---------------------            ----------------------------
   vector<G4InuclEP>                vector<GXDynamicParticle*>
   vector<G4InuclNuclei>
   vector<GXFragment>
```

Class G4InuclCollider

We try to simplify complex inheritance structures

```
** class G4InuclCollider : public G4CascadeColliderBase : public G4VCascadeCollider
- theElementaryParticleCollider:  G4ElementaryParticleCollider*
- theIntraNucleiCascader:         G4IntraNucleiCascader*
- theDeexcitation:                G4VCascadeDeexcitation* theDeexcitation;      // User switchable!
- output:    G4CollisionOutput  // Secondaries from main cascade
- DEXoutput: G4CollisionOutput  // Secondaries from de-excitation

*** InuclCollider::constructor()
+ instantiate theEPCollider [being vectorized]  and theINuclCascader

*** InuclCollider::collide()
+ if(UseEPCollider(bullet,target)) {
    theEPCollider->collide();   <=====  [being vectorized] (more details later)
    return;
  }
+ else { #.. at least one nucleus is present
    (target must always be a nucleus)
    + classify bullet as a hadron or a nucleus (and fill zbullet parameters)
    + boost to TRS (Target Rest System)
    + call theInuclCascader->collide(zbullet, target, output)
    + deexcite then remove recoil fragment
    + boost to LAB frame
    + save final state into output (G4CollisionOutput) object
    + adjust final state kinematics to balance energy and momentum
  }
  + if anything is wrong, call G4CollisionOutput::trivialise()
  return;
```

hadron-hadron collisions
~ 20% of incl. CPU time

hadron-nucleus or
nucleus-nucleus collisions
~ 66% of excl. CPU time

Class G4ElementaryParticleCollider

This class has a large number of non-trivial functions!

Function: collide( )

```
** class G4ElementaryParticleCollider : public G4CascadeColliderBase : public G4VCascadeCollider
*** Constructor: trivial
*** G4ElementaryParticleCollider::collide(bullet, target, output)
+ if(UseEPCollider(bullet, target)) # unnecessary
+ instantiate interCase = InteractionCase(bullet, target)   <== [vectorized]
+ sanity checks
+ instantiate and fill G4LorentzConvertor        <=== [vectorized]
+ boost to center of mass frame                  <=== [vectorized]
+ if a nucleon() is involved, then {             <=== [vectorized]
    if (pionNucleonAbsorption(ekin)) {           <=== [vectorized]
      generateSCMpionNAbsorption(etot_scm, particle1, particle2);   <=== [partly vectorized, not tested]
    } else {
      generateSCMfinalState(ekin, etot_scm, particle1, particle2);  <=== [main function, being vectorized]
    }
  }

+ if a quasi_deutron() is involved {                      <=== [vectorized]
    if (particle1->isMuon() || particle2->isMuon()) {     <=== [vectorized]
      generateSCMmuonAbsorption(etot_scm, particle1, particle2);
    } else {            // Currently, pion absoprtion also handles gammas
      generateSCMpionAbsorption(etot_scm, particle1, particle2);
    }
  }

+ if no valid final state produced so far, return!
+ loop over final state particles
    + boost to Lab frame
+ validate final state for energy and momentum conservation
+ sort FS particles by kinetic energy
+ returns final state particles (output)
```

Plans to re-write these steps with vectorization in mind, to profit from vectorized boosts. Originally, all secondaries are stored in an std::vector.

Class G4ElementaryParticleCollider

Functions: generateSCMfinalState( ), generateMultiplicity( ), generateOutgoingPartTypes( )

```
** class G4ElementaryParticleCollider : public G4CascadeColliderBase : public G4VCascadeCollider
*** Constructor: trivial
*** G4ElementaryParticleCollider::collide(bullet, target, output)...
*** G4ElementaryParticleCollider::generateSCMfinalState(ekin, etot_scm, particle1, particle2)
+ loop to generate valid final state (itry_max = 10)
  + clear output vectors
  + multipl = generateMultiplicity(initState, ekin)          <=== [vectorized]
  + generateOutgoingPartTypes(initState, multipl, ekin)     <=== [vectorizable (imultipl?)]
  + fillOutgoingMasses()   // cache each particle mass, mass2       [vectorized (imultipl?)]
    // Attempt to produce final state kinematics
  + fsGenerator.Configure(particle1, particle2, particle_kinds);      <=== [being vectorized (imultipl?)
  + generate = !fsGenerator.Generate(etot_scm, masses, scm_momentums);  <=== [being vectorized]

+ if any problems, return (no valid final state)
+ store final state particles (and their SCM kinematics)
+ return

*** G4ElementaryParticleCollider::generateMultiplicity(initState, ekin)
+ xsecTable = G4CascadeChannelTables::GetTable(initState);
+ if (xsecTable) multipl = xsecTable->getMultiplicity(ekin);
+ return multipl;

*** G4ElementaryParticleCollider::generateOutgoingPartTypes(initState, multipl, ekin)
+ particle_kinds.clear()          // Initialize buffer for generation
+ xsecTable = G4CascadeChannelTables::GetTable(initState)
+ xsecTable->getOutgoingParticleTypes(particle_kinds, mult, ekin)
+ return particle_kinds
```

Are these possible to be vectorized? *Maybe*, iff multiplicity is homogeneous

Experiment with intra-algorithm re-basketization

G4CascadeFinalStateGenerator class

```
** class GXHadDecayGenerator
*** GXHadDecayGenerator::Generate(G4double initialMass,
                                   const std::vector<G4double>& masses,
                                   std::vector<G4LorentzVector>& finalState)
{
  if (masses.size() == 1U) {
    return GenerateOneBody(initialMass, masses, finalState);
  }
  else {
    theAlgorithm->Generate(initialMass, masses, finalState);
  }
  return !finalState.empty();          // Generator failure returns empty state
}

** class G4CascadeFinalStateGenerator : public GXHadDecayGenerator
*** GXCascadeFinalStateGenerator::Configure(particle1, particle2, particle_kinds)
+ cascadeFinalStateAlg->Configure(bullet, target, particle_kinds)

** class GXVHadDecayAlgorithm
*** GXVHadDecayAlgorithm::Generate(G4double initialMass,
                                    const std::vector<G4double>& masses,
                                    std::vector<G4LorentzVector>& finalState)
{
  // Initialization and sanity check
  finalState.clear();
  if (!IsDecayAllowed(initialMass, masses)) return;

  // Allow different procedures for two-body or N-body distributions
  if (masses.size() == 2U) {
    GenerateTwoBody(initialMass, masses, finalState);     <=== [vectorizable]
  }
  else {
    GenerateMultiBody(initialMass, masses, finalState);   <=== [hard, probably partially vectorizable]
  }
}
```

G4CascadeFinalStateAlgorithm class

```
** class GXCascadeFinalStateAlgorithm : public GXVHadDecayAlgorithm
*** GXCascadeFinalStateAlgorithm::Configure(bullet, target, particle_kinds)
{
  // Identify initial and final state (if two-body) for algorithm selection
  multiplicity = particle_kinds.size();          <=== must be same multiplicity
  G4int is = bullet->type() * target->type();
  G4int fs = (multiplicity==2) ? particle_kinds[0]*particle_kinds[1] : 0;

  ChooseGenerators(is, fs);     <=== probably vectorizable IFF particle_kinds[2] is homogeneous

  // Save kinematics for use with distributions
  SaveKinematics(bullet, target);      <=== [vectorized]

  // Save particle types for use with distributions
  kinds = particle_kinds;
}

*** GXCascadeFinalStateAlgorithm::ChooseGenerators(bullet, target, particle_kinds)
{
  // Choose generator for momentum
  if (G4CascadeParameters::usePhaseSpace()) momDist = 0;
  else momDist = G4MultiBodyMomentumDist::GetDist(is, multiplicity);

  // Choose generator for angle
  if (fs > 0 && multiplicity == 2) {
    G4int kw = (fs==is) ? 1 : 2;
    angDist = G4TwoBodyAngularDist::GetDist(is, fs, kw);
  } else if (multiplicity == 3) {
    angDist = G4TwoBodyAngularDist::GetDist(is);
  } else {
    angDist = 0;
  }
}
```

Several different objects returned depending on is (initial state), fs (final state) and multiplicity