Migrating to the refactored *larg4*

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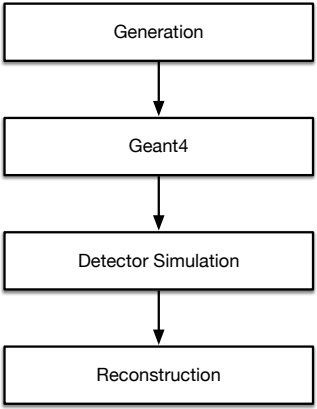
Introduction

- Two options for particle propagation within LArSoft: larsim/LArG4 (legacy) and larg4 (refactored)
- Both interface to Geant4:
  - legacy utilizes a helper class provided by nutools, namely nutools/G4Base (via the G4Helper)
  - refactored utilizes artg4tk

Reference materials:

- nutools/G4Base
- larg4 Wiki
- artg4tk Wiki



LArSoft Simulation chain

Conventions

- larsim/LArG4 will be referred to as Legacy
- the refactored larg4 will be referred to as larg4
- ProtoDUNE Single-Phase will be referred to as PDSP
- Geant4 and G4 will be used interchangeably

Refactored LArG4

Standard – **larsim/LArG4** AKA **Legacy**

- depends on nutools
- ConfigurablePhysicsList.h
- Optical simulation in Legacy was taken out of Geant and adapted from the Peter Gumplinger's original G4 implementations
  - **TheScintillationProcess** → SetScintillationYield()
  - there can be only one scintillating material in the optical simulation (LAr)

Refactored – **LArG4**

- depends on artg4tk (artg4 tool kit)
- Access to reference physics lists + extensions
- Updated OpticalPhysics in G4
  - scintillation properties are attached to the materials
  - can have any number of scintillating materials in the detector (e.g. LAr and plastic scintillator)

See Hans Wenzel's presentation from the DUNE collaboration meeting for a more comprehensive list of features and improvements of the refactored larg4 over Legacy: slides

Goals

- Customization of the physics list tailored to the interest of the physics under investigation
  - Low Energy Physics:
    - Solar Neutrinos
    - Neutron capture
    - Shielding

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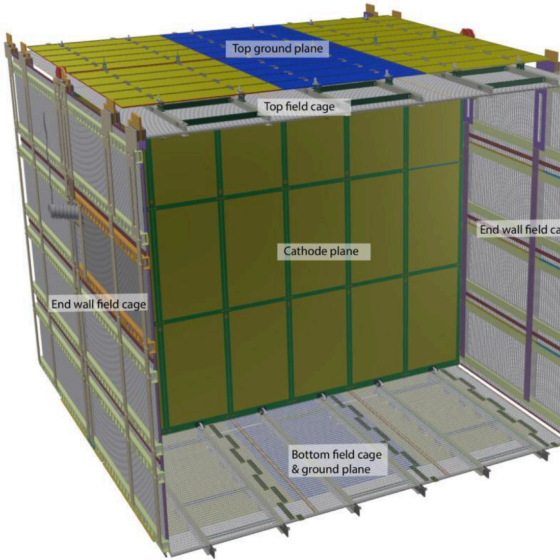
ProtoDUNE Single-Phase

- There is general interest in migrating from legacy to the refactored simulation chain in PDSP
- This is driven mainly by the desire to customize physics lists
- Also, would like to have the ability to do a more *natural* optical simulation with multiple scintillating materials
  - Optical physics within G4 have advanced over the last decade



First Attempt

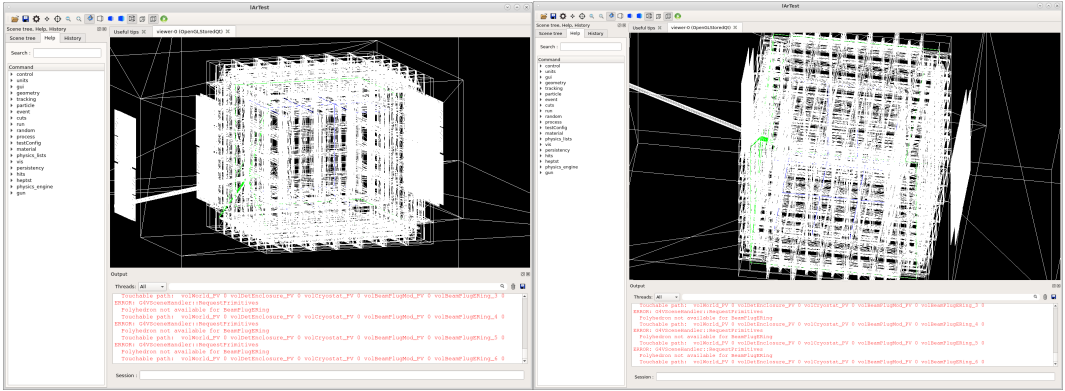
- Hans provided an example refactorization of the 3x1x1 dual-phase detector
  - see Larsoft Feature #22466
- Declared the Liquid Argon volumes as charge sensitive detectors
  - **protodune_v5_refactored.gdml**
  - **protodune_v5_refactored_nowires.gdml**
- Neglected the optical aspect of the simulation, for simplicity
- Redefined the protoDUNE services in the same spirit as the example provided by Hans
- Created corresponding G4→Reconstruction fhicl files
- Also a modified version of the protoDUNE event display fhcil
  - **protoDUNE_refactored_g4.fcl**
  - **protoDUNE_refactored_detsim.fcl**
  - **protoDUNE_refactored_reco.fcl**
  - **evd_refactored_protoDUNE.fcl**

```
967  <structure>
     <volume name="volTPCActive">
       <materialref ref="LAr"/>
       <solidref ref="InnerActive"/>
       <auxiliary auxtype="SensDet" auxvalue="SimEnergyDeposit"/>
       <auxiliary auxtype="StepLimit" auxvalue="0.01"/>
       <auxiliary auxtype="Efield" auxvalue="500."/>
     </volume>
```

Inner Active TPC volume

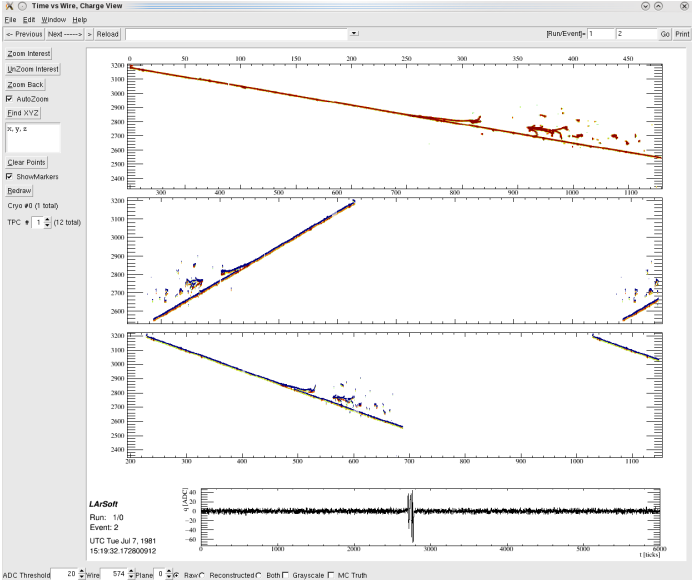
Geometry

- color refs set in the gdml can be visualized in g4



G4 visualization of the protoDUNE v5 geometry generated by H. Wenzel

Example Event : 6GeV μ^-



Example within Larsoft

- The ProtoDUNE migration example can be found on the Redmine Wiki for larg4 : ProtoDUNE Example wiki
- Currently, the ProtoDUNE migration is maintained in a feature branch of dunetpc: **feature/drivera_refactored_larg4_PDSP**
  - Up to date with larsoft v08_22_00

To Do

```xml
<materials>
    <material name="LAr" formula="LAr">
        <property name="RINDEX" ref="ArINDEX"/>
        <property name="SLOWCOMPONENT" ref="SCINT"/>
        <property name="SCINTILLATIONYIELD" ref="SY" />
        <property name="RESOLUTIONSCALE" ref="RS" />
        <property name="SLOWTIMECONSTANT" ref="STC" />
        <property name="YIELDRATIO" ref="YR" />
        <D value="1.40" unit="g/cm3"/>
        <fraction n="1.0000" ref="G4_Ar"/>
    </material>
    <material name="Iron" formula="Iron">
        <property name="RINDEX" ref="ArINDEX"/>
        <D value="4.0" unit="g/cm3"/>
        <fraction n="1.0000" ref="G4_Fe"/>
    </material>
    <material name="Silicon" formula="Si">
        <property name="RINDEX" ref="ArINDEX"/>
        <D value="2.33" unit="g/cm3"/>
        <fraction n="1.0000" ref="G4_Si"/>
    </material>
    <element name="Oxygen"   formula="O"  Z="8.">
        <atom value="16.0"/>
    </element>
    <element name="Nitrogen" formula="N"  Z="7.">
        <atom value="14.01"/>
    </element>
    <element name="Fluorine" formula="F"  Z="9.">
        <atom value="18.9984032"/>
    </element>
    <element name="Lead"     formula="Pb" Z="82.">
        <atom value="207.20"/>
    </element>
    <material name="PbF2">
        <property name="RINDEX" ref="RINDEX"/>
        <D value="7.77" unit="g/cm3"/>
        <composite n="1" ref="Lead"/>
        <composite n="2" ref="Fluorine"/>
    </material>
</materials>
```

Optical material properties

- Define the optical properties of the relevant materials in the geomtry file
- Consider ways to provide physical properties as configuration parameters for the G4 stage
  - E.g. for now the E-field is hard-coded in the geometry file
- Purge refactored services
- Continue validation process
- Compare resource usage between the new and the legacy frameworks

Parting Gifts

The process of adding "new physics" to the Legacy LArG4 is quite convoluted, and prone to breaking changes. Paul Russo and I added the "HadronHP" (High Precision) physics alternative to the standard "Hadron" physics for the purpose of doing Neutron studies. Both handle the hadronic inelastic interactions.

- **HadronHP** – High Precision Inelastic Scattering for hadrons – added to larsim as of Feb. 25
- **HadronElasticHP** – High Precision Elastic Scattering (Neutrons only) (currently in feature branch)
- **HadronElasticPHP** – High Precision Elastic Scattering for various particles (currently in feature branch)

Impressions

- Low barrier of entry concerning the geometry
  - Modifying the GDML file for LArTPC experiments only *requires* specifying the electric field and declaring the Active TPC volume as a **SensitiveDetector**
- Straight-forward to define a separate set of fhicl files that takes advantage of the refactored larg4
  - G4 stage: Only need to become familiar with the Refactored Physics Constructor (artg4tk)
  - Post-G4 stages: Only need to override the SimChannelLabel to match the one for the elecDrift Module (or drift module of your choice)
- At a glance, the physics make a lot more sense
  - Reference physics lists are widely used and are supported by the Geant collaboration

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Neutron Study in Legacy

- Produced various samples of 10 MeV neutrons at the center of TPC1 (larsoft numbering, APA3-active)
- **Issue 1:** simb::MCParticle->EndProcess() for secondary neutrons often returns *FastScintillation*
- **Issue 2:** Some neutrons ending with FastScintillation processes come to rest in the ProtoDUNEFoam
- **Issue 3:** At rest neutrons subsequently decay... ($n \rightarrow p + e^- + \overline{\nu_e}$)
  - Neutron EndProcess is still marked as FastScintillation
  - simb::MCParticle→Process() for proton, e^-, and $\overline{\nu_e}$ returns *Decay*

```
root [16] NeutronAna->Scan("event:((pdg>1E9) ? (pdg-1E9) : pdg):TrackId:Mother:NumberDaughters:G4Process:G4FinalProcess:EndPointx:EndPointy:EndPoin
|| Mother==2) && (G4Process==\"Decay\" || TrackId==2)")
*****************************************************************************************************************************************
*    Row   * Instance *     event * ((pdg>1E9 *   TrackId *    Mother * NumberDau * G4Process * G4FinalPr * EndPointx * EndPointy * EndPointz *
*****************************************************************************************************************************************
*        3 *        1 *         4 *      2112 *         2 *         1 *        61 * neutronIn * FastScint * 17.854642 * 277.86615 * -83.53598 *
*        3 *       68 *         4 *      2212 *        69 *         2 *         0 *     Decay * FastScint * 17.854642 * 277.86615 * -83.53598 *
*        3 *       69 *         4 *       -12 *        70 *         2 *         0 *     Decay * CoupledTr * 1870.1999 * 1778.8261 * -827.6646 *
*        3 *       70 *         4 *        11 *        71 *         2 *         0 *     Decay * FastScint * 17.853923 * 277.33258 * -83.36968 *
*****************************************************************************************************************************************
```

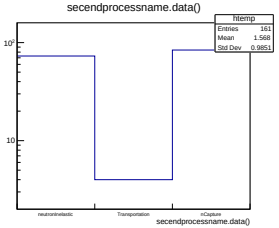
G4 Printout

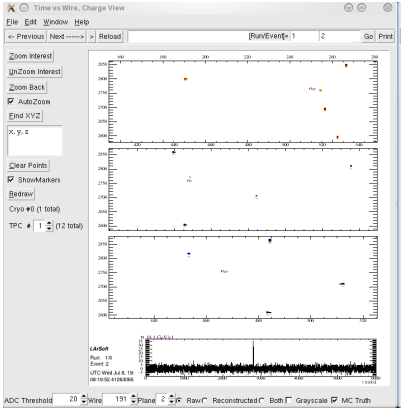
```
From G4:
     ********************************************************************************************
     * G4Track Information:   Particle = neutron,   Track ID = 18,   Parent ID = 12
     ********************************************************************************************

     Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
         0 -1.49e+03 4.39e+03      832     0.172        0        0         0 volTPCActiveInner_PV initStep
         1 -1.46e+03  4.4e+03      768     0.158        0     72.3      72.3 volTPCActiveInner_PV hadElastic
         2 -1.45e+03 4.39e+03      788     0.146        0     23.3      95.6 volTPCActiveInner_PV hadElastic
....
        86 -1.74e+03 5.82e+03     -643  3.43e-11        0     64.1  1.65e+04 volFoamPadding_PV hadElastic
        87 -1.72e+03 5.87e+03     -621  2.82e-11        0     53.8  1.65e+04 volFoamPadding_PV hadElastic
        88 -1.75e+03 5.86e+03     -604         0        0     30.8  1.65e+04 volFoamPadding_PV hadElastic
    |   89 -1.75e+03 5.86e+03     -604         0        0        0  1.65e+04 volFoamPadding_PV FastScintillation
```

Revisiting the Neutron Simulations in refactored larg4

- Disabled Neutron time-based cut
- Using the same gen stage input Root file, ran it through the refactored simulation chain
- Selected QGSP_BERT_HP reference physics list
- No more neutron decays!





EndProcess for secondary neutrons produced in 10MeV neutron events simulated in the refactored framework

Refactored Physics Constructor

```
artg4tk::PhysicsListService::PhysicsListService(fhicl::ParameterSet const & p, art::ActivityRegistry &) :
  PhysicsListName_( p.get<std::string>("PhysicsListName","FTFP_BERT")),
  DumpList_( p.get<bool>("DumpList",false)),
  enableNeutronLimit_(p.get<bool>("enableNeutronLimit",true)),
  NeutronTimeLimit_(p.get<double>("NeutronTimeLimit",10.*microsecond)),
  NeutronKinELimit_(p.get<double>("NeutronKinELimit",0.0)),
  enableStepLimit_(p.get<bool>("enableStepLimit",true)),
  enableOptical_(p.get<bool>("enableOptical",true)),
  enableCerenkov_( p.get<bool>("enableCerenkov",false)),
  CerenkovStackPhotons_( p.get<bool>("CerenkovStackPhotons",false)),
  CerenkovMaxNumPhotons_(p.get<int>(" CerenkovMaxNumPhotons",100)),
  CerenkovMaxBetaChange_(p.get<double>("CerenkovMaxBetaChange",10.0)),
  CerenkovTrackSecondariesFirst_( p.get<bool>("CerenkovTrackSecondariesFirst",false)),
  enableScintillation_( p.get<bool>("enableScintillation",true)),
  ScintillationStackPhotons_( p.get<bool>("ScintillationStackPhotons",false)),
  ScintillationByParticleType_( p.get<bool>("ScintillationByParticleType",true)),
  ScintillationTrackInfo_( p.get<bool>("ScintillationTrackInfo",false)),
  ScintillationTrackSecondariesFirst_( p.get<bool>("ScintillationTrackSecondariesFirst",false)),
  enableAbsorption_( p.get<bool>("enableAbsorption",false)),
  enableRayleigh_( p.get<bool>("enableRayleigh",false)),
  enableMieHG_( p.get<bool>("enableMieHG",false)),
  enableBoundary_( p.get<bool>("enableBoundary",false)),
  enableWLS_( p.get<bool>("enableWLS",false)),
  BoundaryInvokeSD_( p.get<bool>("BoundaryInvokeSD",false)),
  verbositylevel_( p.get<int>("Verbosity",0)),
  WLSProfile_( p.get<std::string>("WLSProfile","delta"))
{}
```

OpFastScintillation

```
324   ////////////
  1   // Methods
  2   ////////////
  3
  4 // AtRestDoIt
  5 // ----------
  6 //
  7   G4VParticleChange*
  8   OpFastScintillation::AtRestDoIt(const G4Track& aTrack, const G4Step& aStep)
  9
 10   // This routine simply calls the equivalent PostStepDoIt since all the
 11   // necessary information resides in aStep.GetTotalEnergyDeposit()
 12
 13   {
 14     return OpFastScintillation::PostStepDoIt(aTrack, aStep);
 15   }
 16
 17 // PostStepDoIt
 18 // ------------
 19 //
 20   G4VParticleChange*
 21   OpFastScintillation::PostStepDoIt(const G4Track& aTrack, const G4Step& aStep)
 22   // This routine is called for each tracking step of a charged particle
 23   // in a scintillator. A Poisson/Gauss-distributed number of photons is
 24   // generated according to the scintillation yield formula, distributed
 25   // evenly along the track segment and uniformly into 4pi.
 26
 27   {
 28     aParticleChange.Initialize(aTrack);
 29
 30     // Check that we are in a material with a properties table, if not
 31     // just return
 32     const G4Material* aMaterial = aTrack.GetMaterial();
 33     G4MaterialPropertiesTable* aMaterialPropertiesTable =
 34       aMaterial->GetMaterialPropertiesTable();
 35     if (!aMaterialPropertiesTable)
 36       return G4VRestDiscreteProcess::PostStepDoIt(aTrack, aStep);
 37
 38     G4StepPoint* pPreStepPoint  = aStep.GetPreStepPoint();
 39
 40     G4ThreeVector x0 = pPreStepPoint->GetPosition();
 41     G4ThreeVector p0 = aStep.GetDeltaPosition().unit();
```