Geant4 Condensed Matter Package

From the SuperCDMS Detector Monte Carlo Group

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What is G4CMP?

Library built on top of Geant4 to add support for low energy condensed matter physics.

Some Features:

- Awareness of various crystal symmetries (and amorphous solids)
- Transport and interactions of (acoustic) phonons
- Transport and interactions of charge carriers (electrons and holes)
- Support for local electric fields from 3D potential maps.
- Seamlessly transition from "normal" Geant4 energy deposits to G4CMP particle physics.

Using G4CMP

Install from GitHub.com,

```
git clone https://github.com/ragnese/g4cmp
```

Set up Geant4 environment as usual.

Add **G4CMPPhysicsList** and a **G4LatticePhysical** to your application.

Link application to libG4CMP.{so,a} and then G4. (Order matters!)

Lattice Configuration

G4LatticeLogical - Physics properties

- Crystal symmetry group, lattice constants
- Stiffness tensor
- Electron/hole effective masses, conduction band "valley" directions
- Scattering rates/parameters

G4LatticePhysical - Orientation of G4LatticeLogical

- Attaches to G4VPhysicalVolume
- Owns G4LatticeLogical (calls through for physics params)
- Crystal orientation from Miller indices and rotation angles

Using G4Lattice{Logical,Physical}

```
G4VPhysicalVolume* G4DMCDetectorConstruction::Construct() {
[...]

// Load the lattice for the material we're using
G4LatticeManager* latManager = G4LatticeManager::GetLatticeManager();
G4Material* germanium = nistManager->FindOrBuildMaterial("G4_Ge");
latManager->LoadLattice(germanium, "Ge"); // latManager has LogicalLattice info

// Define our detector volume as usual
G4VSolid* germaniumSolid = new G4Tubs("germaniumCyl", 0.*cm, 3.81*cm,
                                      zipThickness/2., 0.*deg, 360.*deg);
G4LogicalVolume* germaniumLogical = new G4LogicalVolume(zipSolid, germanium,
                                                        "germaniumLogical");
G4VPhysicalVolume* germaniumPhysical = new G4PVPlacement(0, DMCcoords,
                                                         germaniumLogical,
                                                         "germaniumPhysical",
                                                         worldLogical,
                                                         false, 0);

// Attach a physical lattice to our physical volume
G4LatticePhysical* detLattice = new G4LatticePhysical(latManager->GetLattice(germanium));
detLattice->SetMillerOrientation(1,0,0,0.);
// Register pVol <-> pLat relationship for look up by processes
latManager->RegisterLattice(pv, detLattice);

[...]
}
```

Configuration Files

Germanium

```
# Crystal parameters
cubic 5.658
stiffness 1 1 1.26e11
stiffness 1 2 0.44e11
stiffness 4 4 0.67e11
# Phonon parameters
beta -0.732 gamma -0.708
   lambda 0.376 mu 0.561
scat 3.67e-41
decay 1.6456e-54
LDOS 0.097834
STDOS 0.53539
FTDOS 0.36677
# Charge carrier parameters
vsound 5324.2077
l0_e 257e-6
l0_h 108e-6
# Hole and electron masses
hmass 0.350
emass 1.588 0.081 0.081
valley  -45 35.2644 90 deg
valley   45 35.2644 90 deg
valley  135 35.2644 90 deg
valley -135 35.2644 90 deg
# Intervalley scattering
ivField 217
ivRate 6.72e-2
ivPower 3.24
```

Silicon

```
# Crystal parameters
cubic 5.431
stiffness 1 1 1.656e11
stiffness 1 2 0.639e11
stiffness 4 4 0.795e11
# Phonon parameters
beta -0.429 gamma -0.945
   lambda 0.524 mu 0.680
scat 2.43e-42
decay 7.41e-56
LDOS  0.093
STDOS 0.531
FTDOS 0.376
# Charge carrier parameters
vsound 9000.0
l0_e 16.9e-6
l0_h 7.5e-6
# Hole and electron masses
hmass 0.50
emass 0.91 0.19 0.19
valley   0  0 90 deg
valley  90  0 90 deg
valley   0 90 90 deg

# Intervalley scattering
ivField 217
ivRate 6.72e-2
ivPower 3.24
```

```
# angstrom (Lattice constant)
# C11, C12, C44 in Pa


# S. Tamura et al., PRB31(4), 1985
# 10\^11 Pa

# s\^3
# s\^4
# S. Tamura et al., PRB44(7), 1991


# m/s (approximate)
# m
# m

# per m(electron)
# per m(electron)
# Euler angles phi,theta,psi


# V/m
# s (Using Ge rate for Si for now)
# exponent in sqrt(field^ivPower)
```

Physics Processes

Mode mixing (due to isotope scattering)

Anharmonic decay (L $\rightarrow$ L$'$ T, L $\rightarrow$ T T)

Intervalley scattering (no $\vec{k}$ change, just v $\rightarrow$ v$'$ index)

Luke-Neganov phonon emission (discrete, one step per emission)

Boundary processes á là **G4OpBoundaryProcess**

- Specify absorption, reflection, transmission probabilities
- Thresholds for absorption, total reflection
- Can fill HitCollection for digitization, sensor simulation
- If **G4CMPVElectrodePattern** is attached to surface, absorb under specified conditions

Particle Kinematics

Non-Newtonian (non-SR) kinematics, not G4 compatible

Geant4 Assumes:

- $E^2 = p^2 + m^2$
- $\hat{v} = \hat{p}$
- if (m == 0) v = c;

G4CMP Needs:

- Phonon $\vec{k}$ vs. $\vec{v}_g$; m=0, $v \neq c$
- Electrons have m_{ij} tensor
- Brillouin valleys, Herring-Vogt space

Particle Kinematics

G4CMP processes **CAN NOT** use the usual G4Track accessors: GetMomentum(), GetKineticEnergy(), etc.

G4CMPProcessUtils Implements the necessary helpers: GetMomentum(G4Track*), etc. Also applies to filling the ParticleChange.

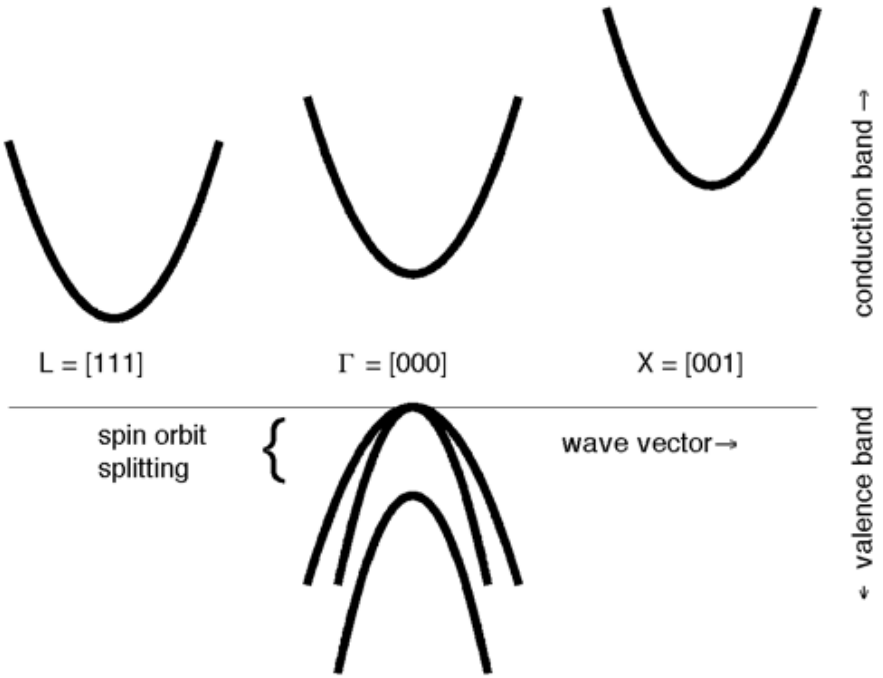
G4CMP uses **G4AuxiliaryTrackInformation** to store and retrieve extra kinematic quantities for each track (e.g. wave vector direction of phonons)

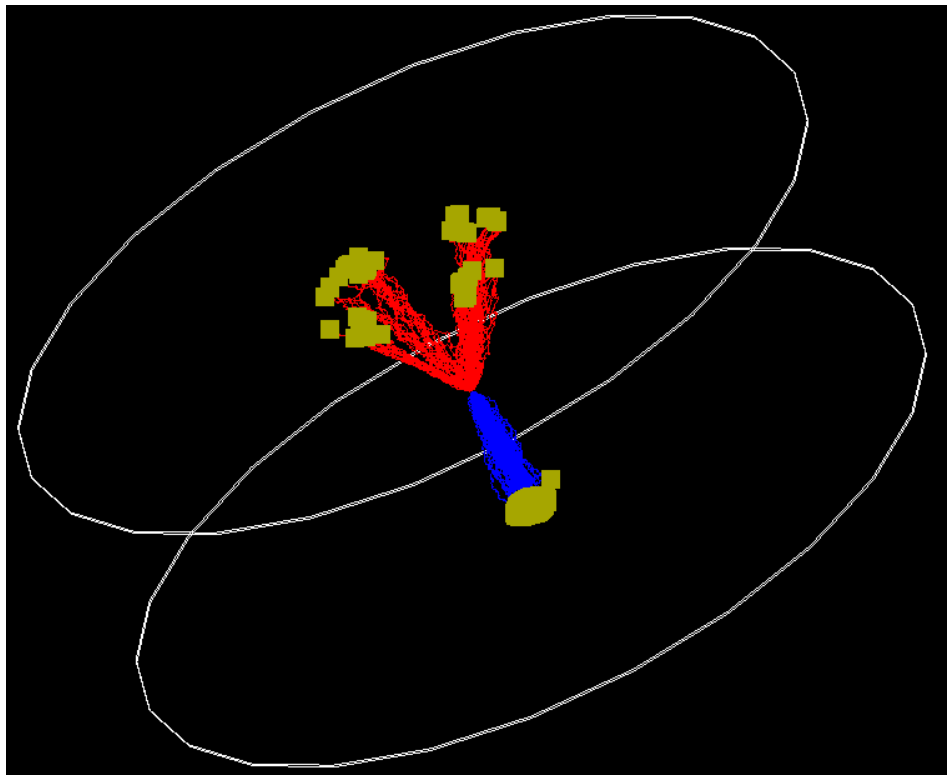
G4CMPStackingAction populates TrkInfo for generated primaries

Secondaries created with TrkInfo filled automatically by inheriting from **G4VPhononProcess** or **G4CMPVDriftProcess**

Charge Carrier Propagation

G4CMP uses a tensor effective mass for transportation of charges

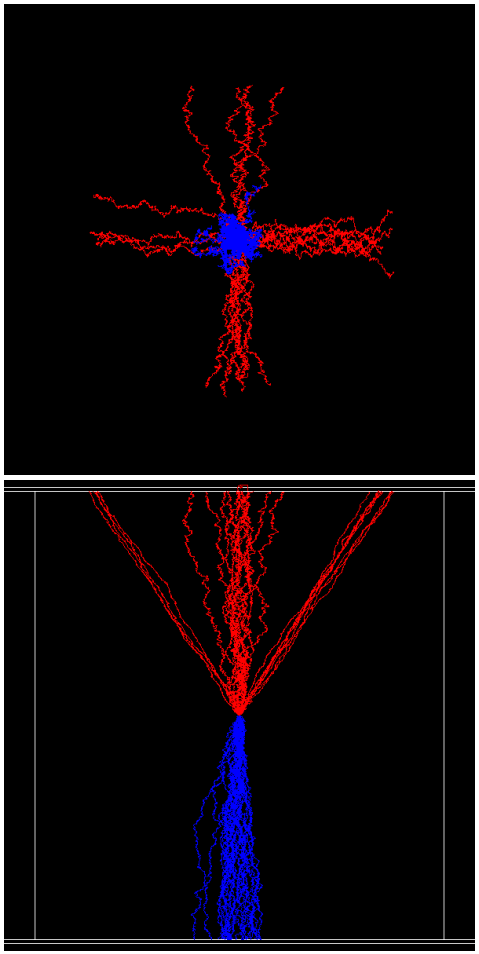




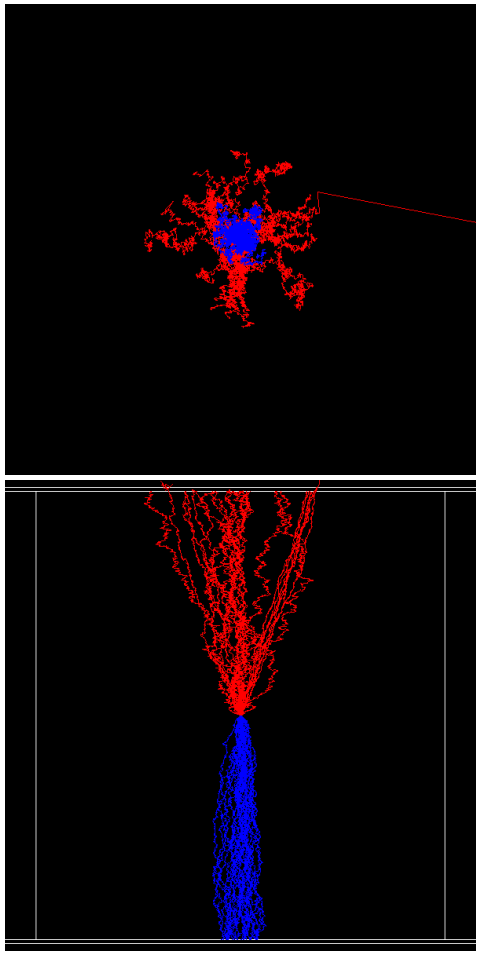
Electron Trajectories

76×25 mm crystals, uniform 4 V field, no IV scattering

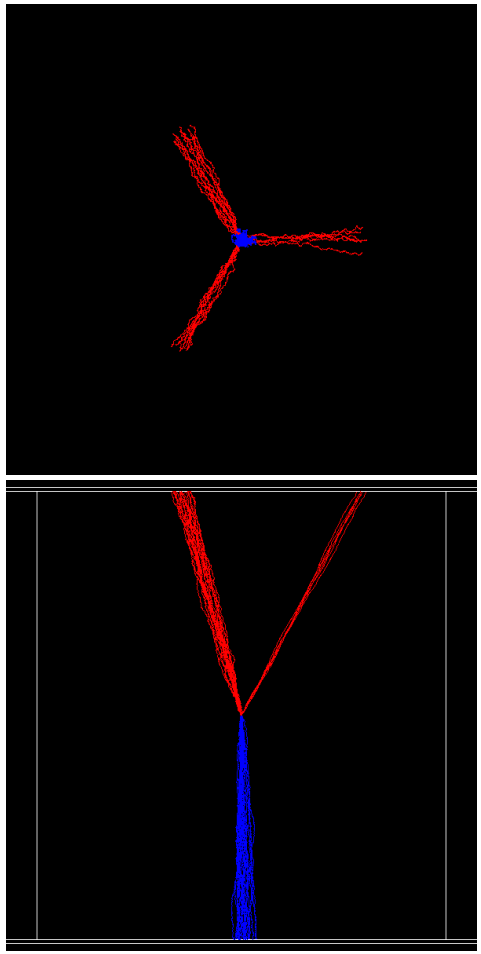
Ge (100)



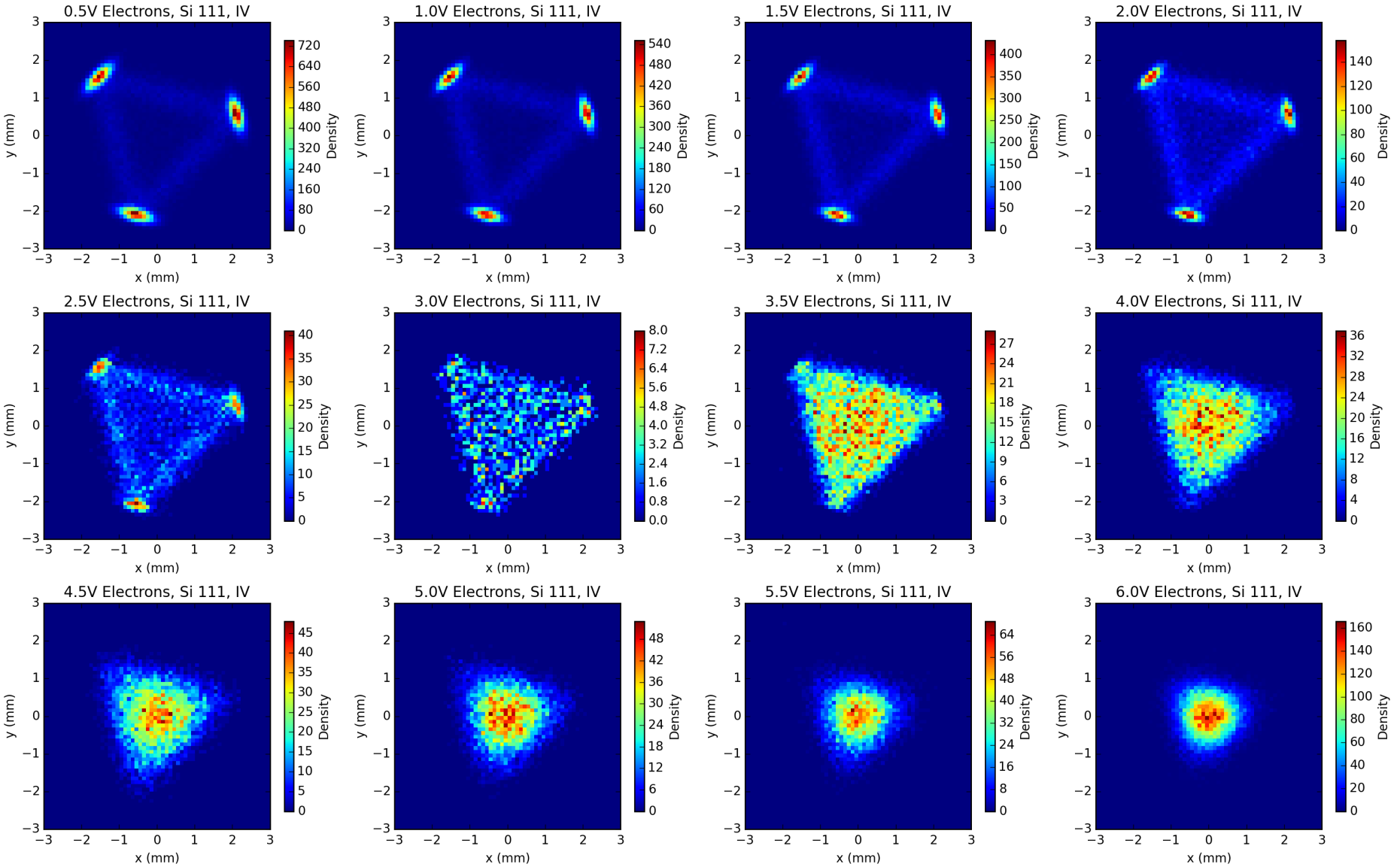
Ge (111)



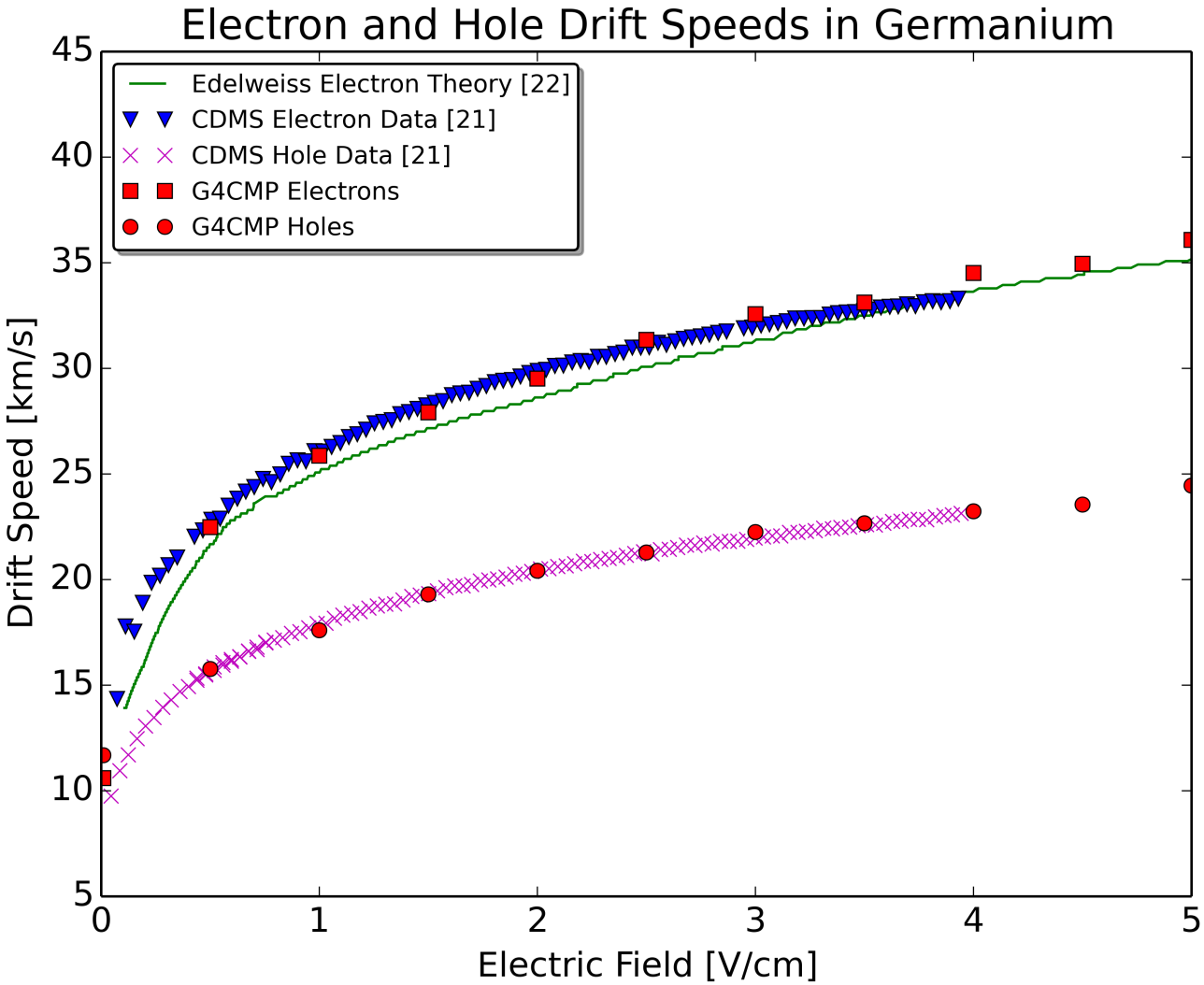
Si (111)



Electron Hits in Silicon (111)



Charge Carrier Drift Speed



Phonon Propagation

Phonon mode m (L, ST, FT), wavevector $\vec{k}$, $\hat{n} = \vec{k}/|k|$

Compute Christoffel matrix $D_{ik} = n^j n^l C_{ijkl}$

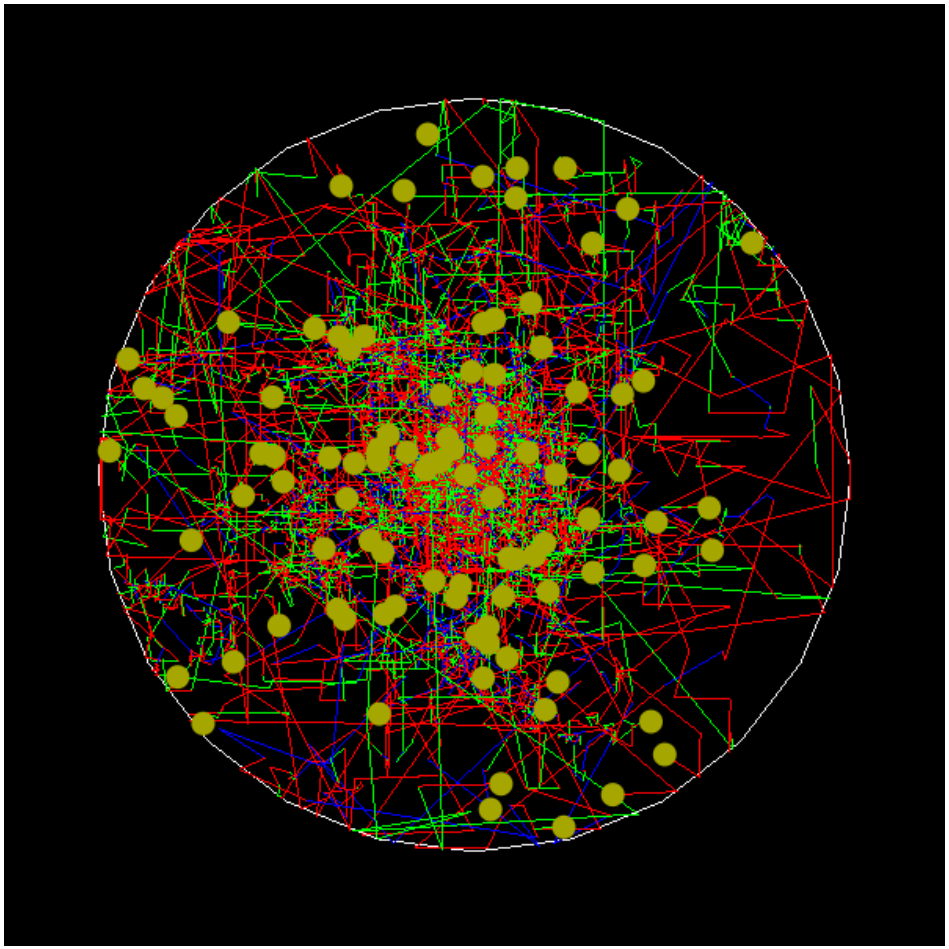
Use eignvector solver on D_{ik}

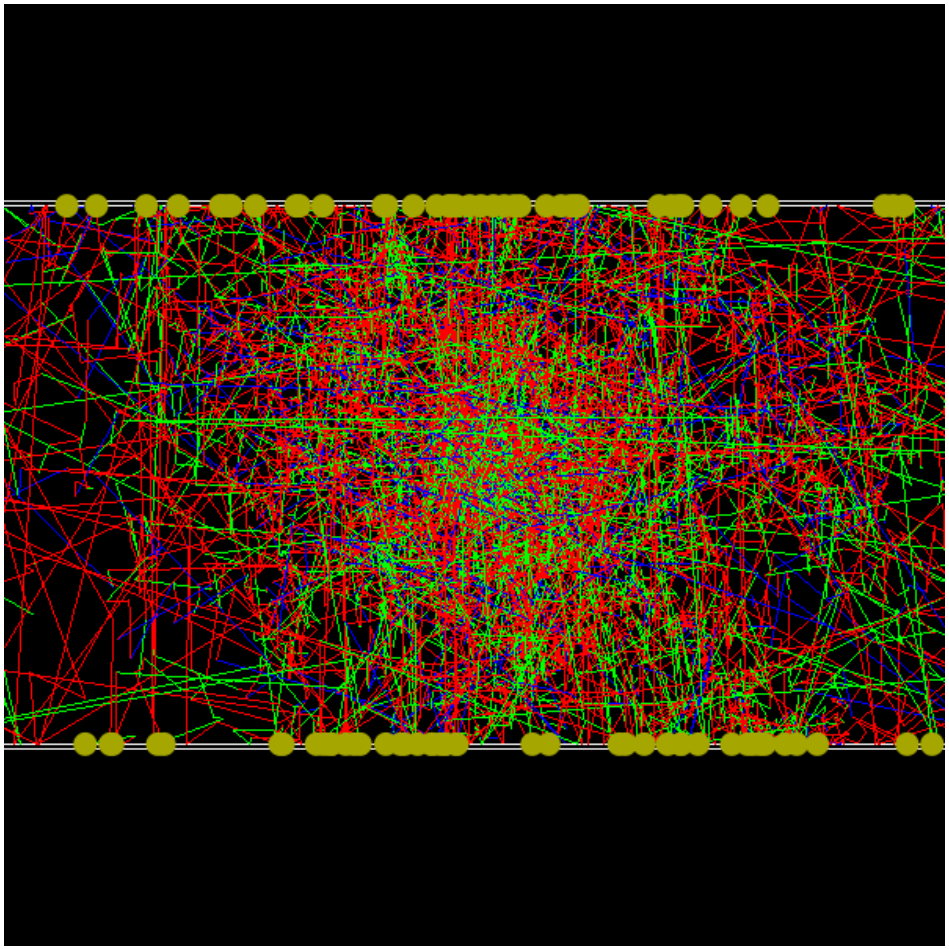
- Eigenvalues are phase speeds $v_s^{(m)}$
- Eigenvectors are true polarizations $\vec{e}^{(m)}$
- Group velocities extracted including material density ρ
  $\vec{v}_{g,l}^{(m)} = \frac{1}{\rho v_s} e^{(m),i} n^j e^{(m),k} C_{ijkl}$

Solver not fast enough to use during running ($\times 3$ lookup)

Populate lookup tables in $\hat{n}$ (ϕ, θ) by **G4LatticeLogical** ctor

Phonons in Germanium





What's New in 2016?

- Support for crystal symmetries other than simple cubic
- Lattice config file for Si (already had Ge)
- Support for sensitive electrode patterns at boundaries (G4CMPVElectrodePattern)
- Charges recombine and release bandgap energy at rest
- Phonons reflect (optionally) diffusely from surfaces
- Kaplan quasi-particle downconversion for phonons that absorb in a superconductor NOTE: The quasi-particles are not actually simulated
- Utilize Geant4 track biasing by weight
- User configurable minimum cutoff energies
- Lindhard partitioning of energy deposits to create primaries/secondaries

Symmetry Groups

Group	Arguments	Stiffness Components Cpq
cubic	*a*	C11 C12 C44
tetragonal	*a c*	C11 C12 C13 C16
		C33 C44 C66
orthorhombic	*a c*	C11 C12 C13 C22
		C23 C33 C44 C55 C66
hexagonal	*a b c*	C11 C12 C13 C33 C44 C66
rhombohedral	*a* α `deg|rad`	C11 C12 C13 C14 C15
		C33 C44 C66
monoclinic	*a b c* α `deg|rad`	orthorhombic +
		C45 C16 C26 C36
triclinic	*a b c* α β γ `deg|rad`	All 21 Cpq
amorphous	none	C11 C12

Energy Partitioning For New Tracks

G4CMPEnergyPartition uses Lindhard theory to partition deposited energy between phonons and charges. Adapted from Lewin And Smith, 1996:

$$\epsilon = 0.0115E \times Z^{-7/3}$$

$$k = 0.133\frac{Z^{2/3}}{\sqrt{A}}$$

$$h = \epsilon + 0.7\epsilon^{0.6} + 3\epsilon^{0.15}$$

$$LindhardFactor = \frac{kh}{1+kh}$$

Also applies the Fano factor from the crystal to vary the number of charge carrier pairs created.

G4CMPSecondaryProduction is a continuous process that picks up all energy depositions from **non-G4CMP** particle tracks and uses **G4CMPEnergyPartition** to spawn G4CMP secondaries.

TODO

Add more materials

Add support for optical phonon modes

Convert Luke phonon emission to a continuous process

Use more experimental data to validate/tune various parameters (e.g., recombination phonon distribution)

Create Bogoliubov quasiparticle type for tracking through superconductors