G4CMP: Condensed Matter Physics Simulations with GEANT4

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G4CMP: Condensed Matter Physics Simulation Using the GEANT4 Toolkit

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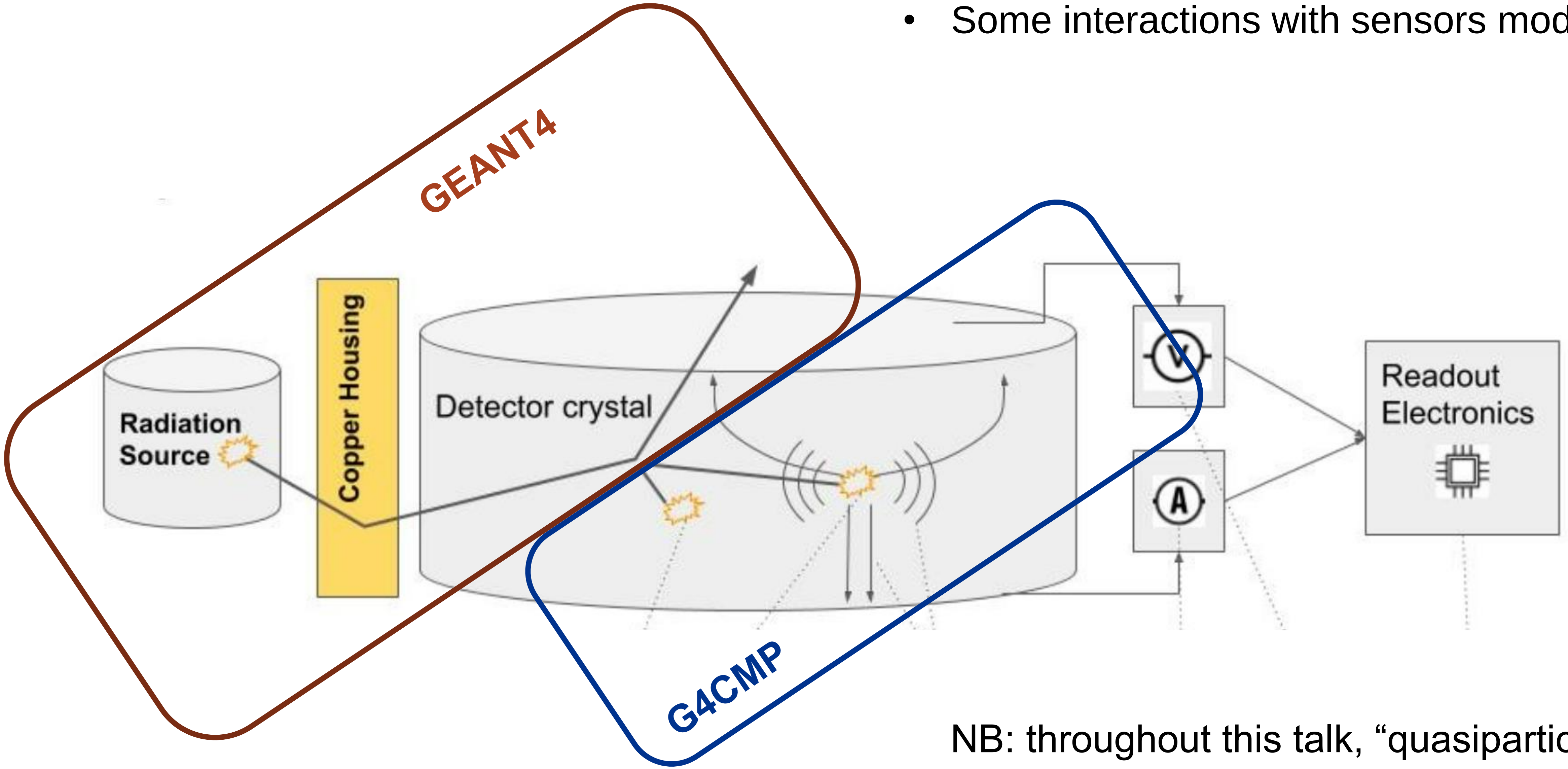
Outline

- What is G4CMP?
- Example applications
- Physics processes modeled in G4CMP
  - Charge transport
  - Phonon transport
  - Superconducting electrodes
- How to use

What is G4CMP?

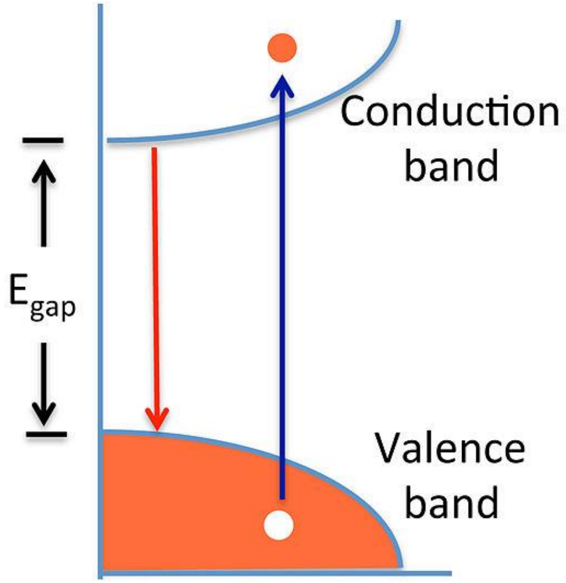
- G4CMP takes energy deposits from GEANT4 to produce and then track e/h pairs and phonons
- Can use detailed 2D or 3D electric field meshes
- Some interactions with sensors modeled



NB: throughout this talk, "quasiparticle" refers to ½ of a broken Cooper pair in a superconductor

What is G4CMP?

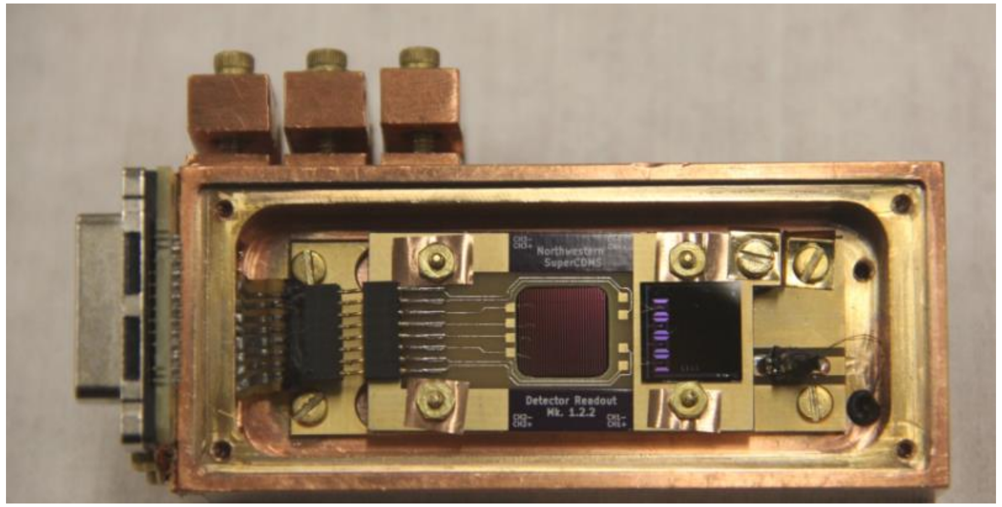
- Software library that extends GEANT4 particle transport to include phonons and electron/hole pair propagation in semiconductor crystals
- Models *athermal, transient* excitations
- Similar in some ways to treatment of optical photons in GEANT4:
  - Based on well-understood condensed matter physics models
  - but requires many empirical values especially for surface interactions
- Built-in parameterizations for Ge and Si
  - Still need to specify parameters like charge trapping mean free paths

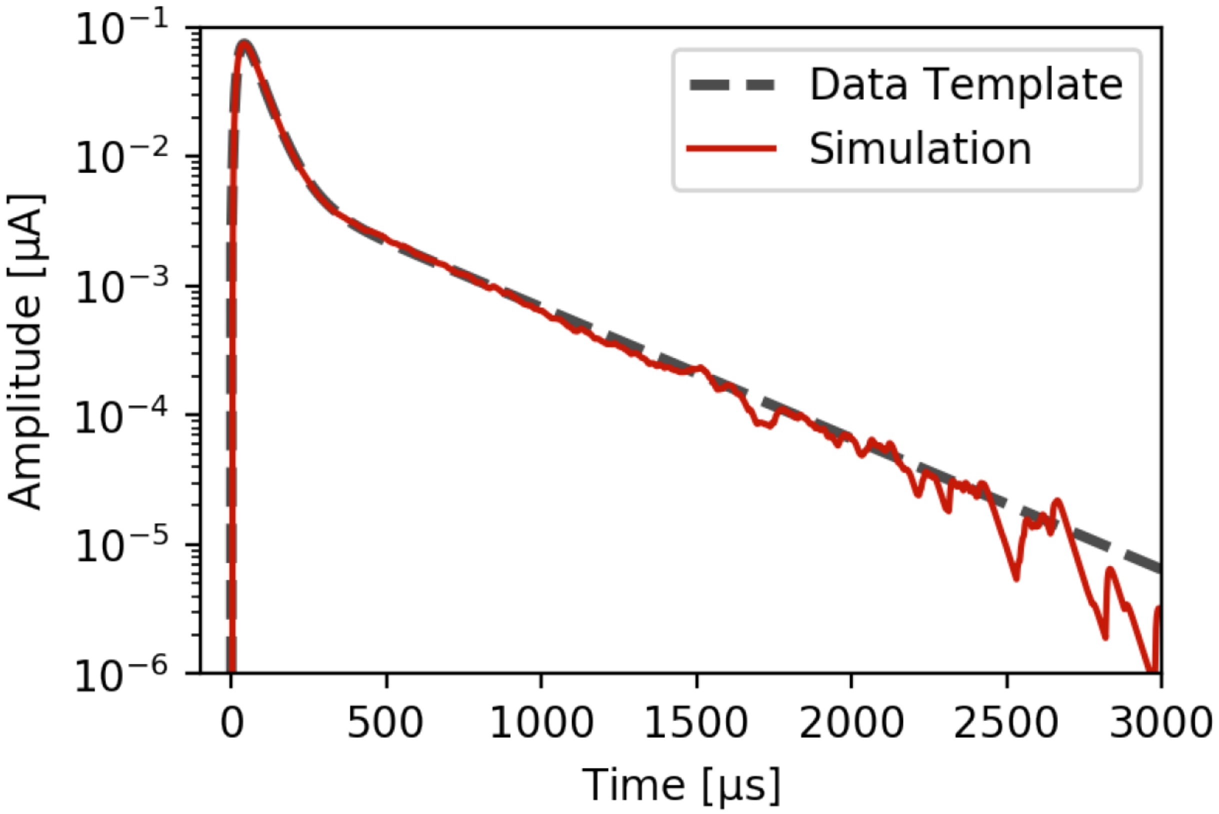


Application examples

Sensor response time profile

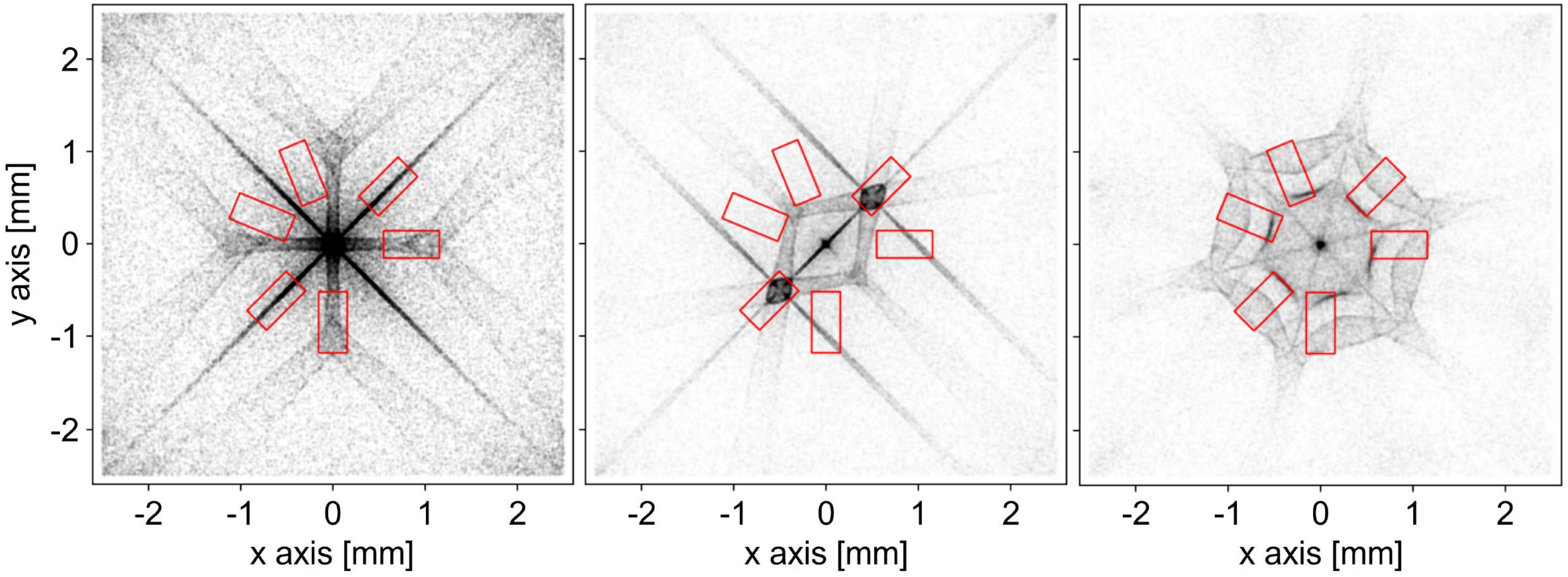
- Response time of SuperCDMS HVeV detector to optical photon pulses
- Early time matches data well out-of-the box
- Late fall time requires parameter tuning, some to non-physical values
- Most likely culprits are no quasiparticle diffusion model, and no modeling of bolometric heat transfer to fridge bath





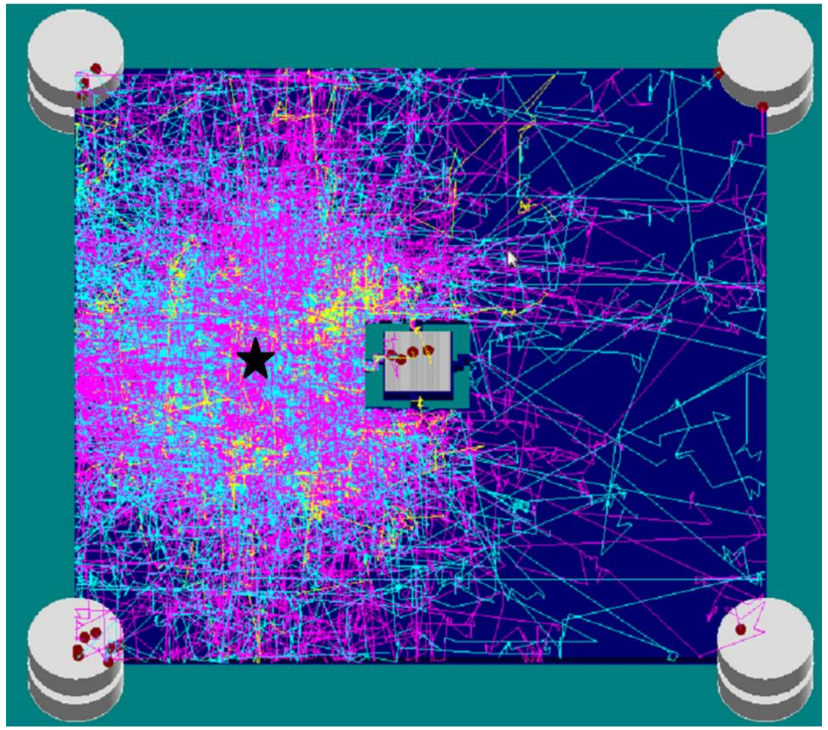
Optimizing phonon sensor placement

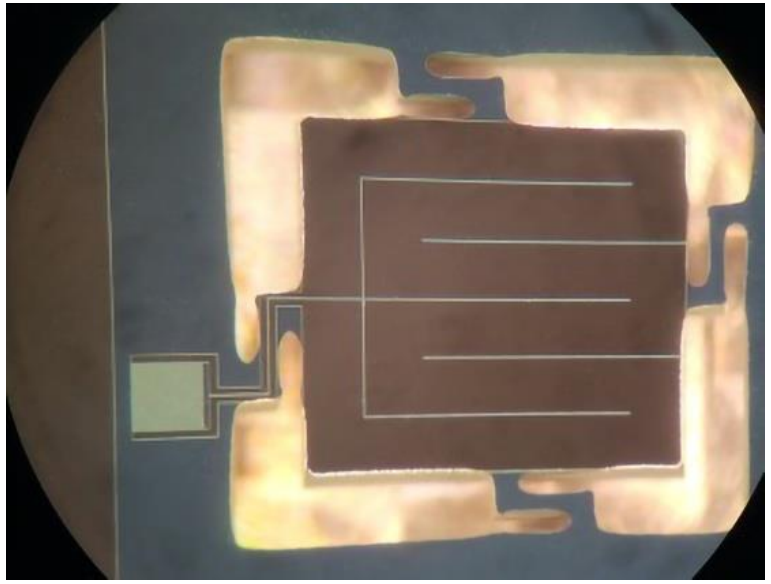
- Localized energy inputs lead to phonon caustics depending on crystal orientation
- Red boxes are suggested locations for sensors designed to measure the caustics explicitly
- More generally sensor placement could be tuned for maximum absorption or position sensitivity

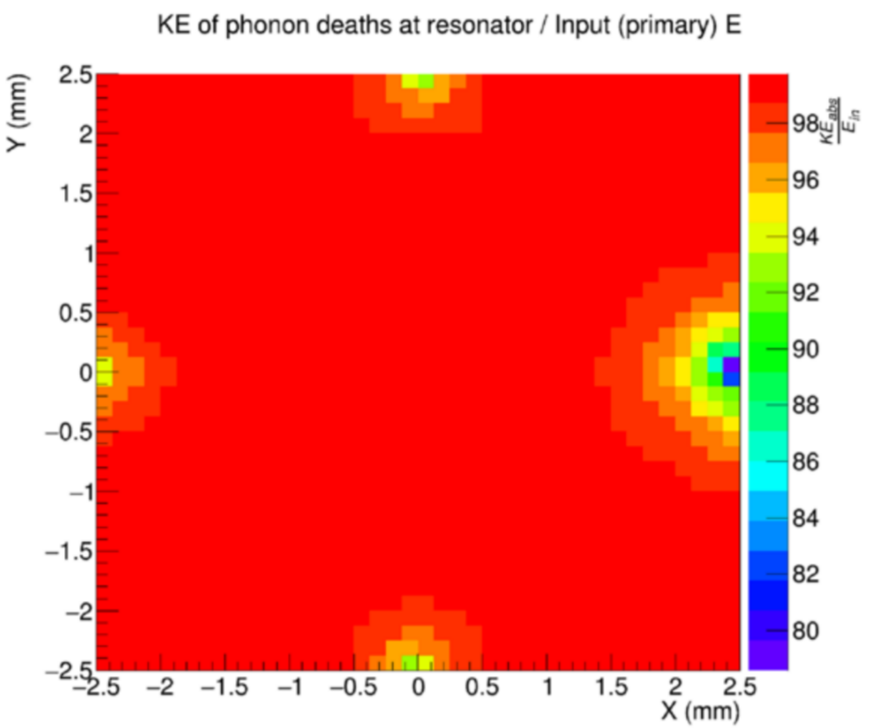


Trenching for sensor isolation

- Sensitive devices like qubits want to be isolated from energy input to the larger substrate
- Conversely bolometers want to contain energy in small island -> larger temperature increase
- G4CMP simulated leakage of phonons into and out of island isolated with micro-machined legs

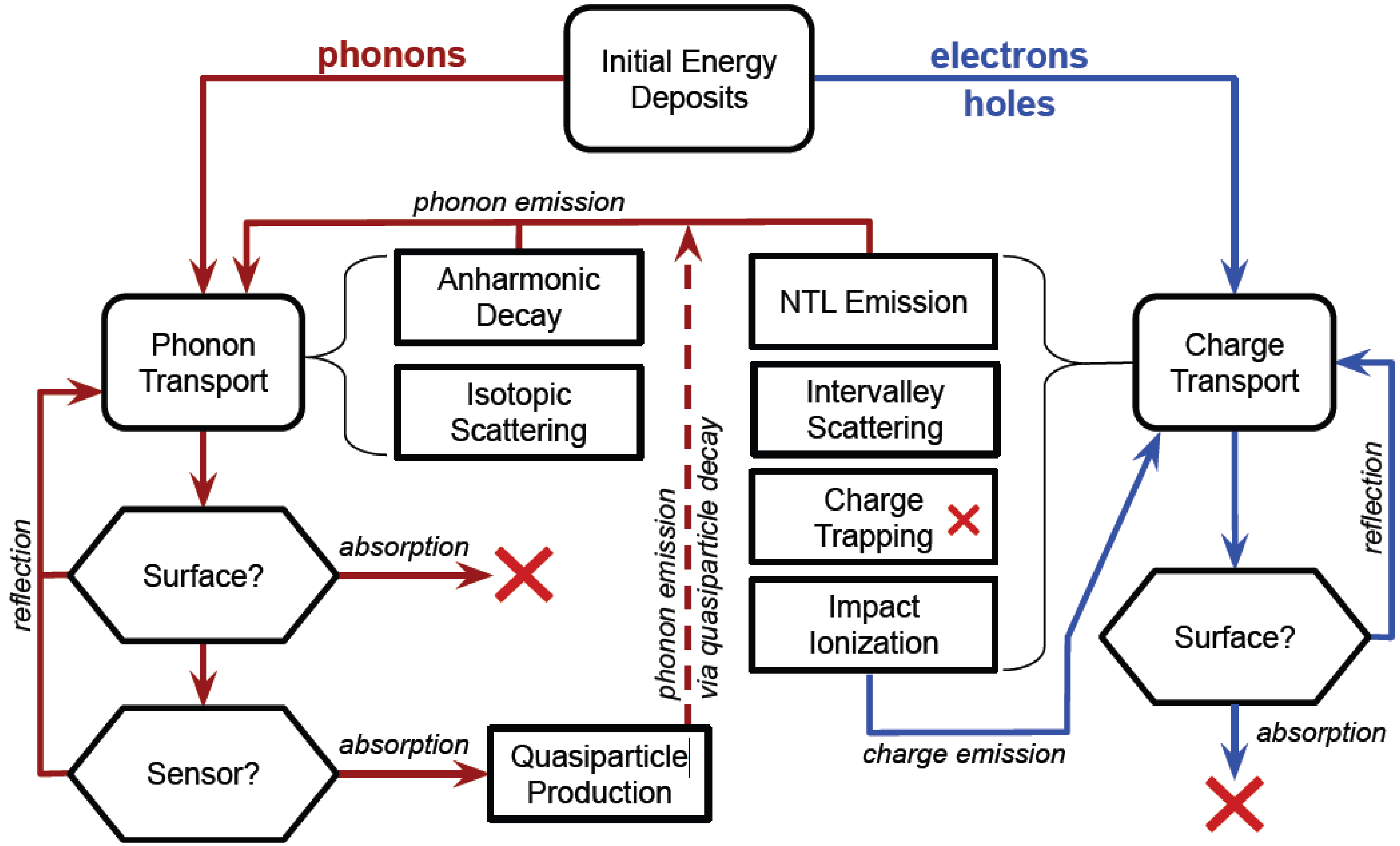






$z_{primary}$=-800um, 'planar' particle gun geometry

G4CMP physics processes

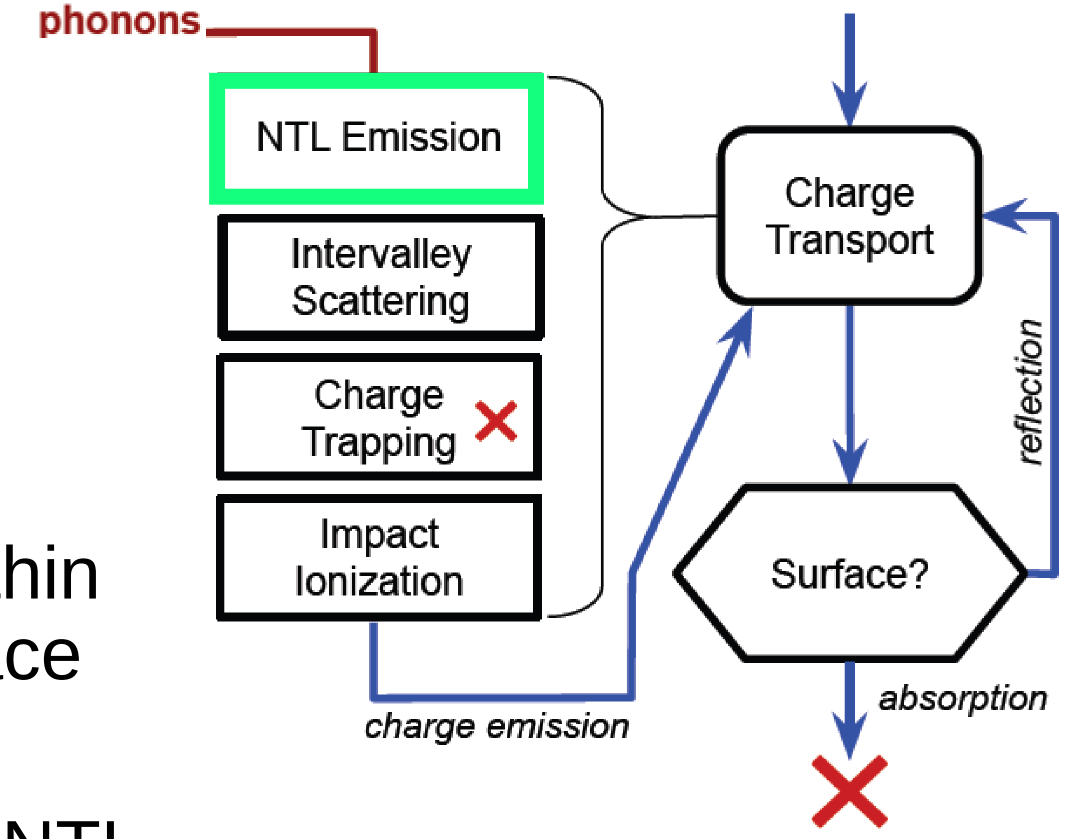


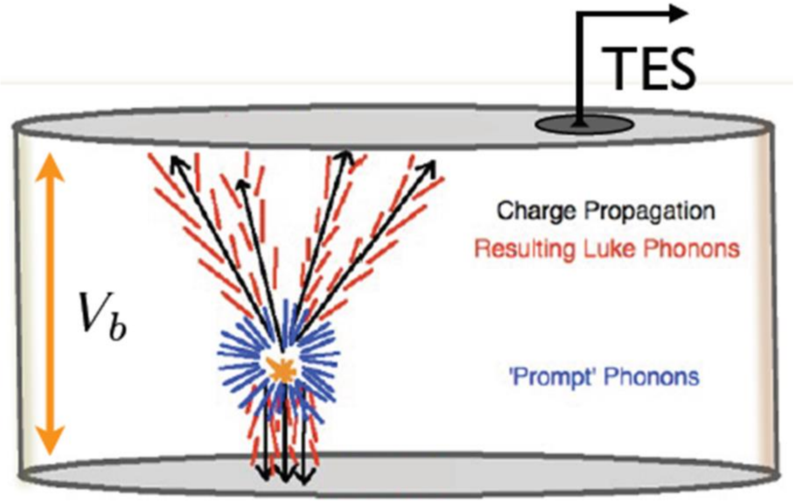
Initial excitation creation

- Electromagnetic energy deposited all goes into creation of e/h pairs
  - $N_{avg} = E_{dep} / E_{avg}$ (3.81 in Si), sampled from Poisson-like distribution with Fano factor (F~0.15 in Si)
  - Each particle given same energy E_{dep}/N
- Energy deposited by heavy ions or nuclear recoils partitioned into primary phonons and e/h pairs based on yield model (default Lindhard)
  - All phonons start with approximately Debye energy
  - No optical phonons modeled, assumed to immediately downconvert to acoustic phonons

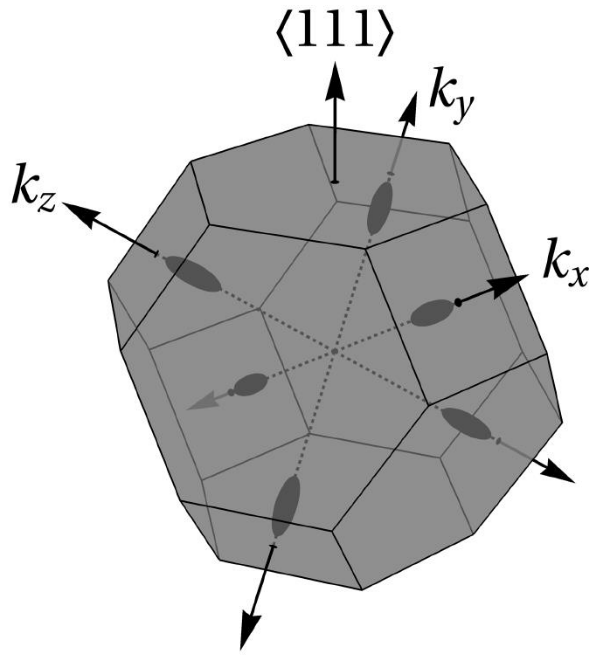
Charge propagation: NTL emission

- Supersonic charges shed energy by emitting phonons, analogous to Cerenkov radiation
- At zero electric field, primary e/h lose energy within ~microns and then continue until they hit a surface
- With electric field, charge carriers reach steady-state average drift speed and continuously emit NTL phonons
- This property enables SuperCDMS HV detectors to reach low thresholds
- Total phonon emission = 1 eV / V / pair
  - For 50 eV energy deposit, npairs = 13.1
  - At 100V bias, total measured energy will be 50eV + 13.1 * 100eV = 1.36 keV





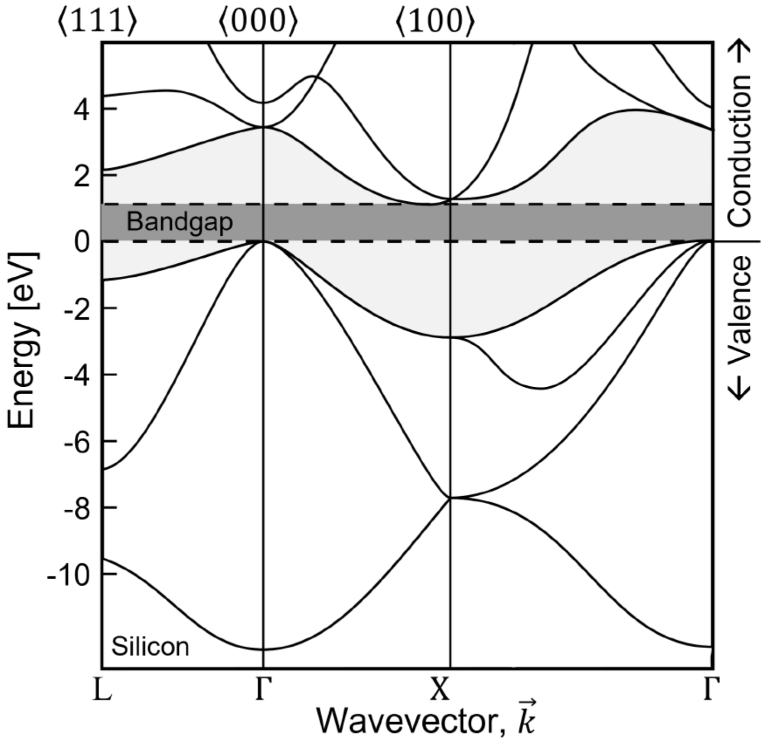
Oblique charge propagation and inter-valley scattering



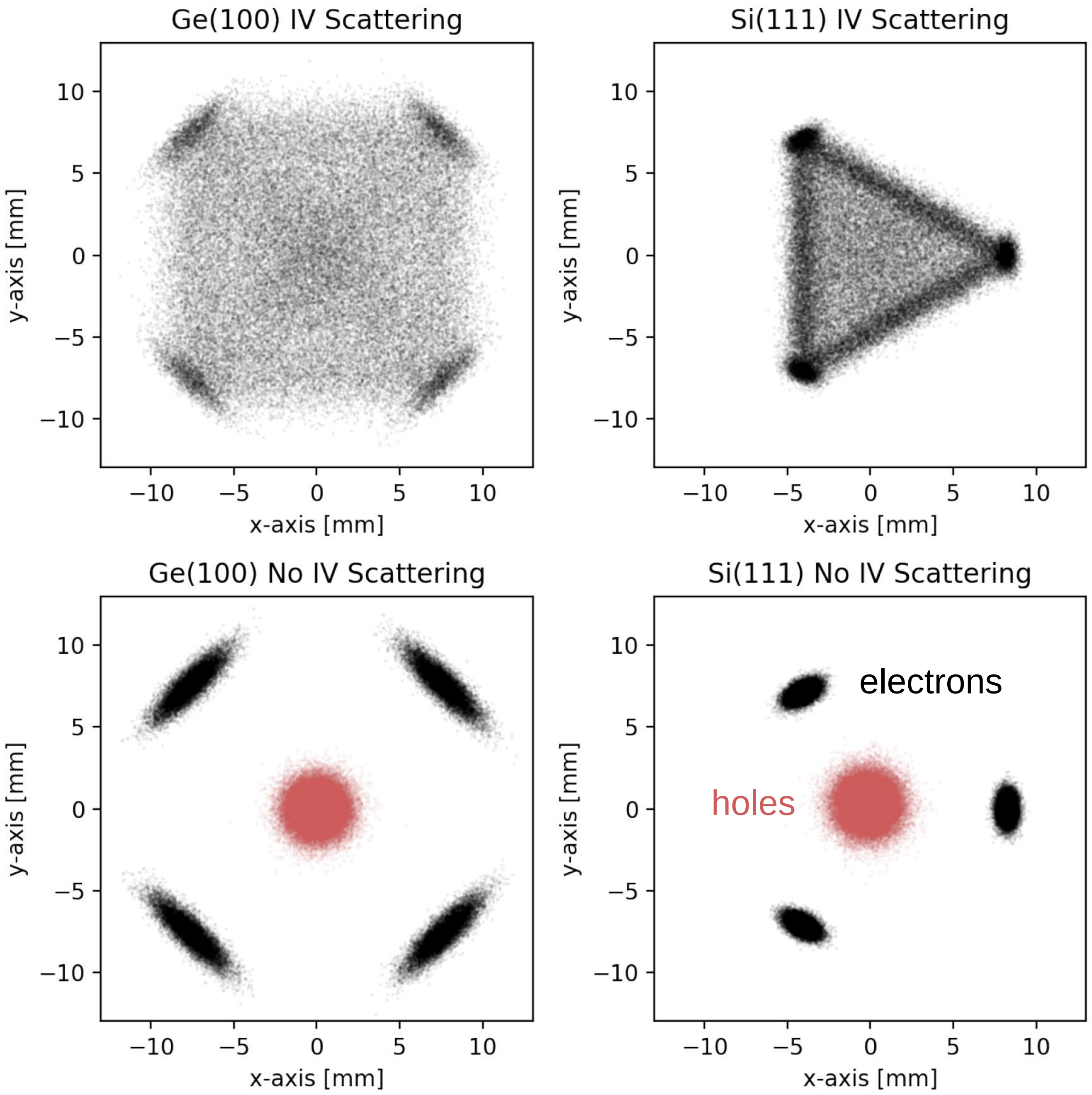
- Holes propagate isotropically at zero field, or follow field lines, ignoring crystal orientation
- Electrons have preferred minimum-energy propagation directions not aligned with typical wafer crystal orientation
- Can scatter off the lattice or impurities to rotate into a different valley propagation direction
- Rate can be parameterized with linear or quadratic forms in electric field

$$\nu_{IV} = b + m|\vec{E}|^{\alpha} \qquad \nu_{IV} = A\left(E_0^2 + |\vec{E}|^2\right)^{\alpha/2}$$

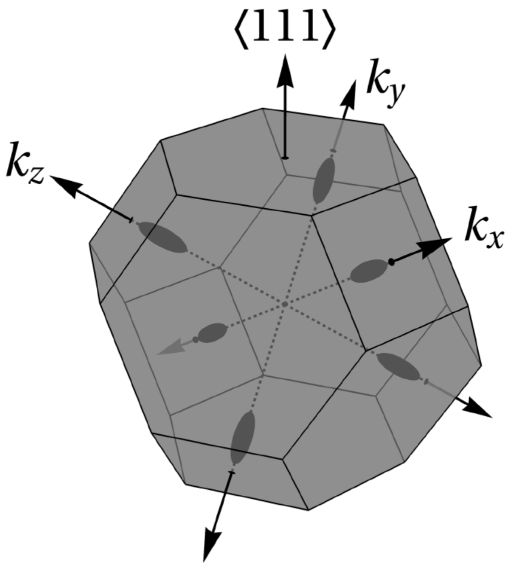
- Default parameterization for silicon scales as E^4



Inter-valley scattering



- Valleys lead to distinct charge collection patterns from point sources
- IV scattering smears result
- NTL emission broadens all distributions including holes



Charge carrier drift speed

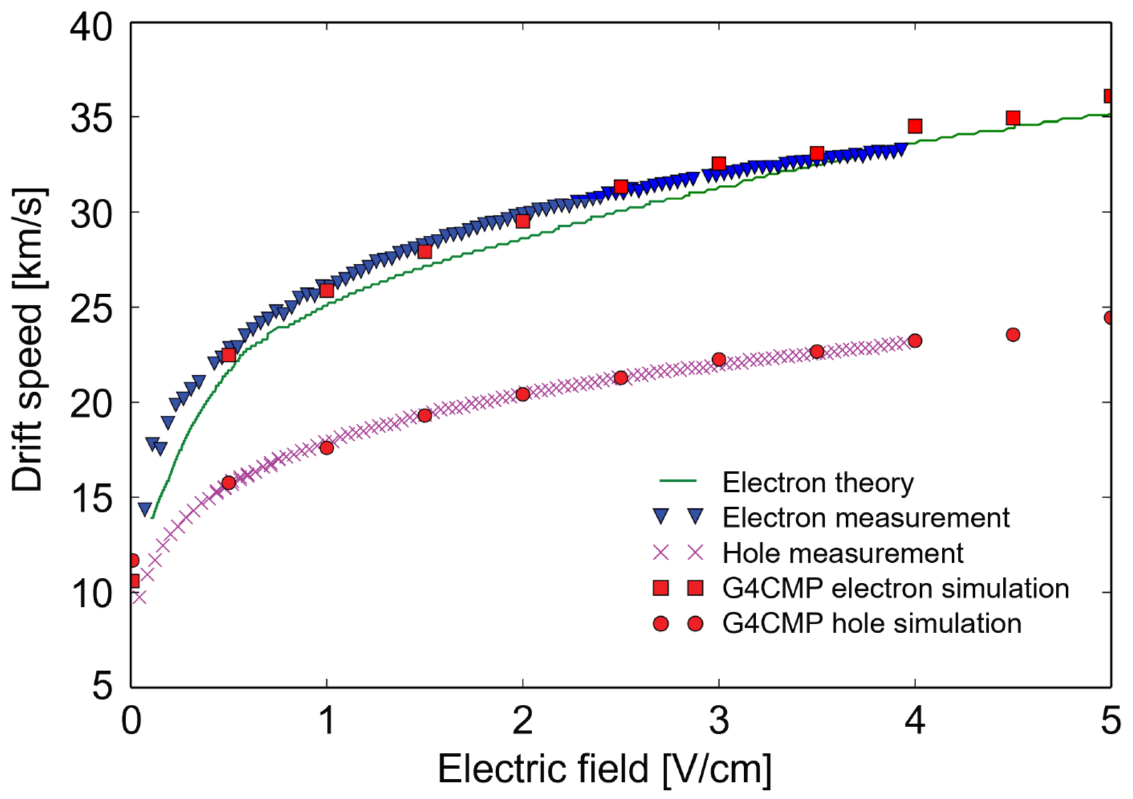
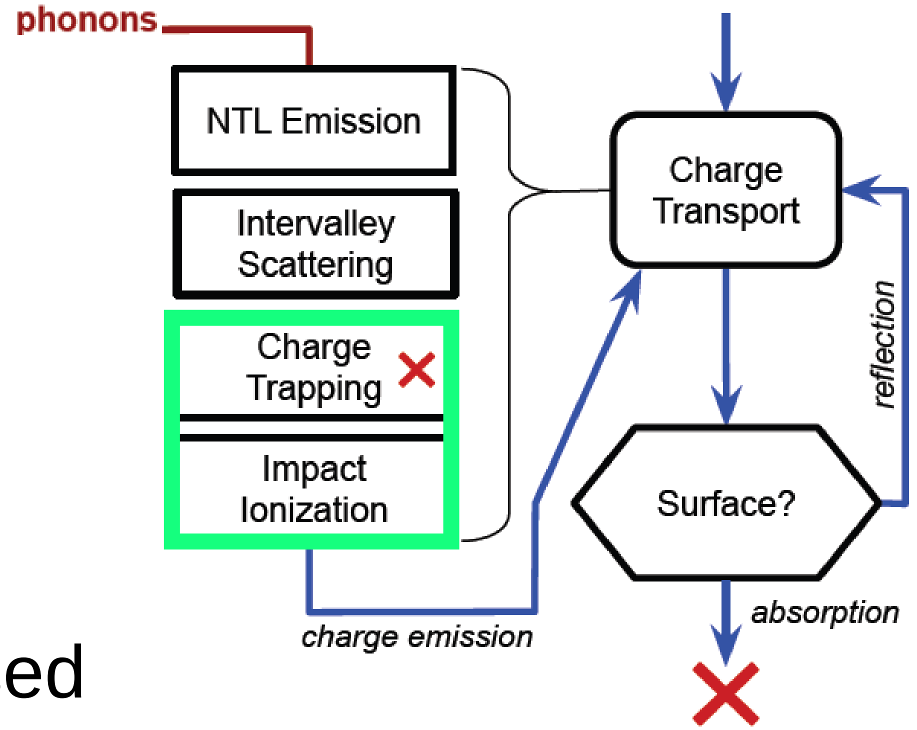
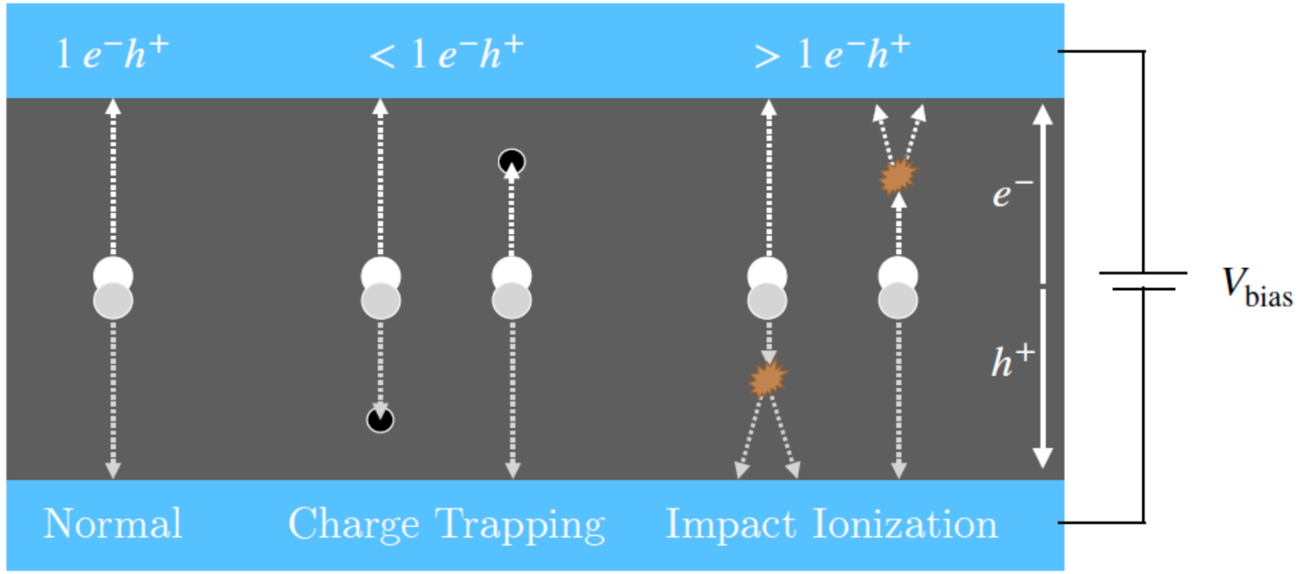


Figure 7: G4CMP-simulated drift speeds in Ge versus applied electric-field strength for electrons (red squares) and holes (red circles), compared to experimental data from Ref. [60] for electrons (blue triangles) and holes (magenta ×'s) and to the theoretical model from Ref. [63] (green curve). Figure adapted from Ref. [2].

Charge trapping and impact ionization

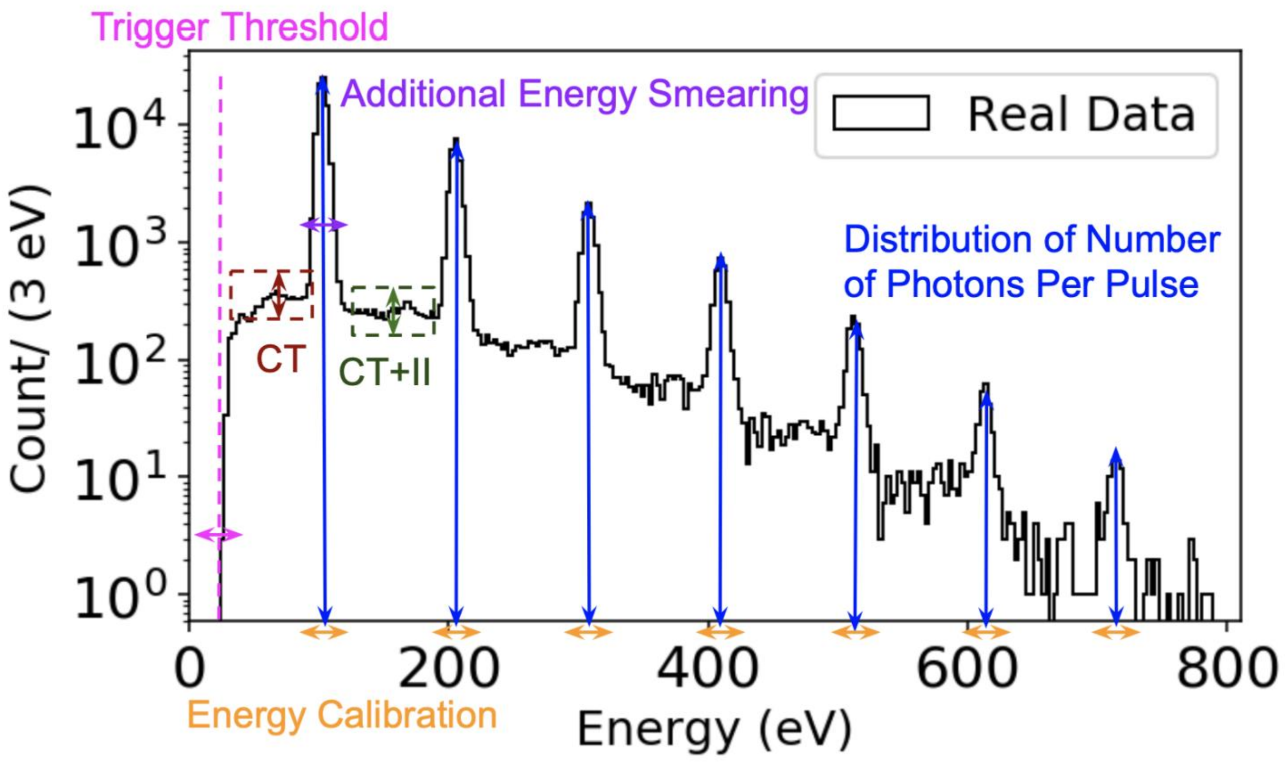
- e/h interactions with impurities in crystal
- Assume impurities create local potential wells much smaller than bandgap
- Trapping -> charge is lost
- Impact ionization -> previously trapped charge released
- Only e or h produced, promotion of a pair from valence band (e.g. avalanche diode) takes much larger field and not modeled
- Highly device dependent, default disabled

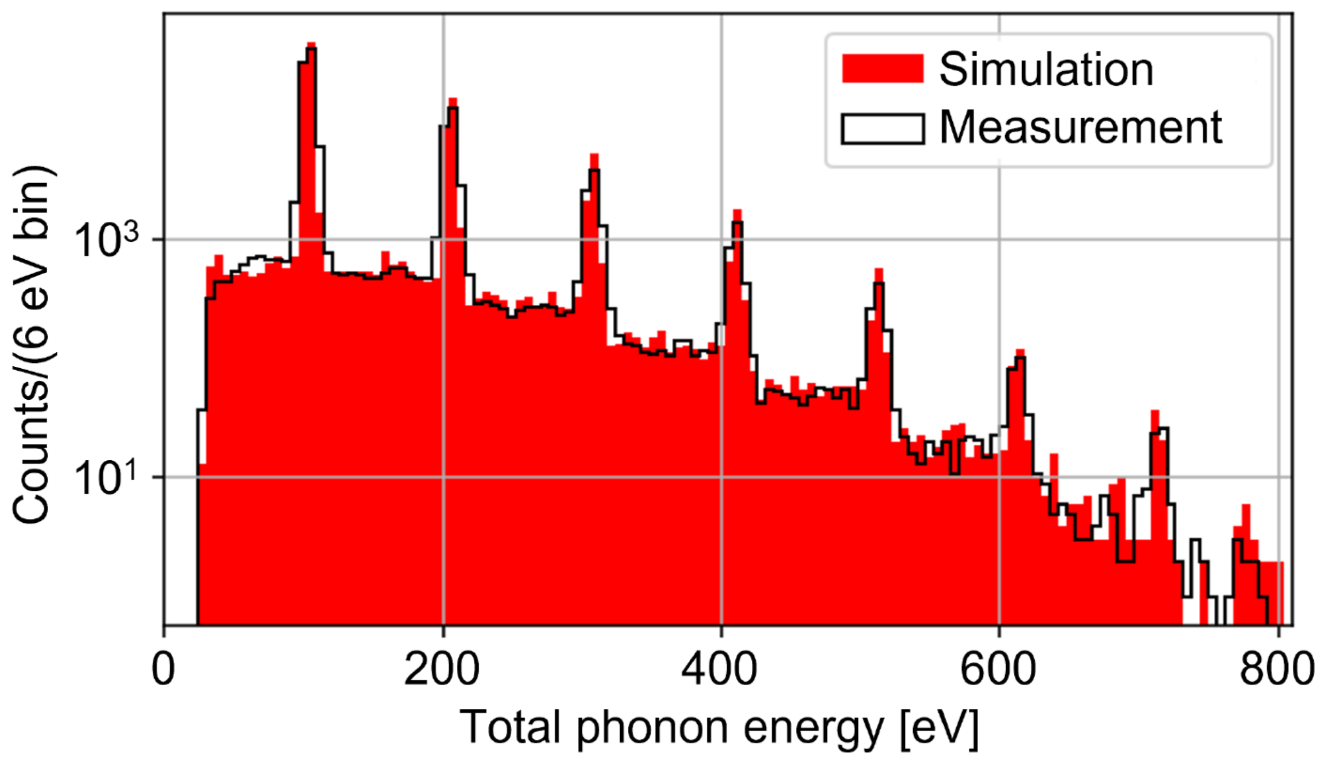




Charge trapping and impact ionization

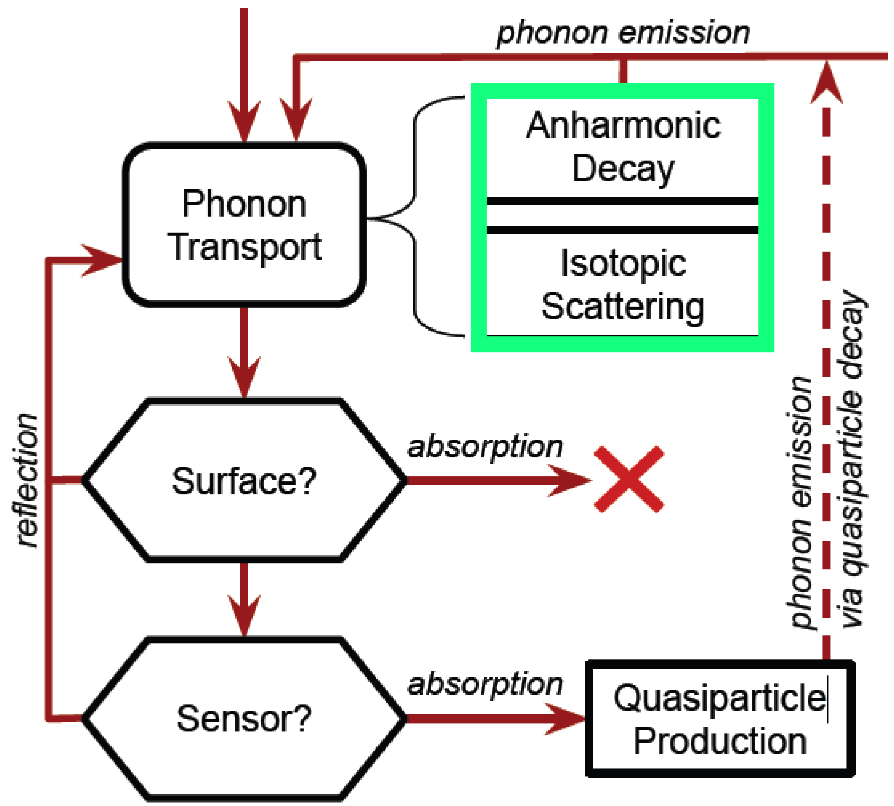
- With electric field, charge trapping and impact ionization lead to ~flat fill between e/h peaks
(since interaction can happen anywhere along field direction)





E. Azadbakht, Comparison of Simulations and Data from Small High Voltage Single Crystal Detectors for Dark Matter Searches, Ph.D. thesis, Texas A&M University (2022). www.slac.stanford.edu/exp/cdms/ScienceResults/Theses/azadbakht.pdf

Phonon processes



- Optical (high energy) phonons not modeled, assume immediately downconvert to low energy acoustic modes
  - No phonon-photon interactions
- Acoustic can downconvert to two lower-energy phonons by anharmonic decay, exchanging momentum with the lattice
  - Rate proportional to E^5
- Can also scatter into random direction and polarization (mode mixing) keeping same energy off isotopic substitution site
  - Rate proportional to E^4
- High energy phonons highly diffusive, typically downconvert over ~micron lengths then become ballistic (~cm scattering lengths)

Phonon Propagation

- Anisotropic phonon propagation leads to focusing into caustics patterns

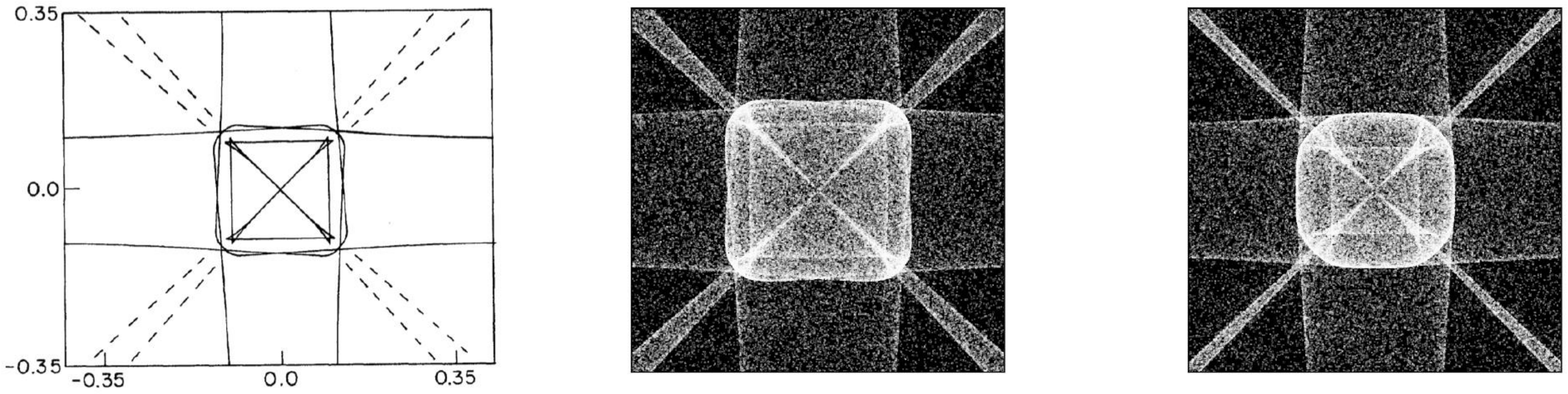
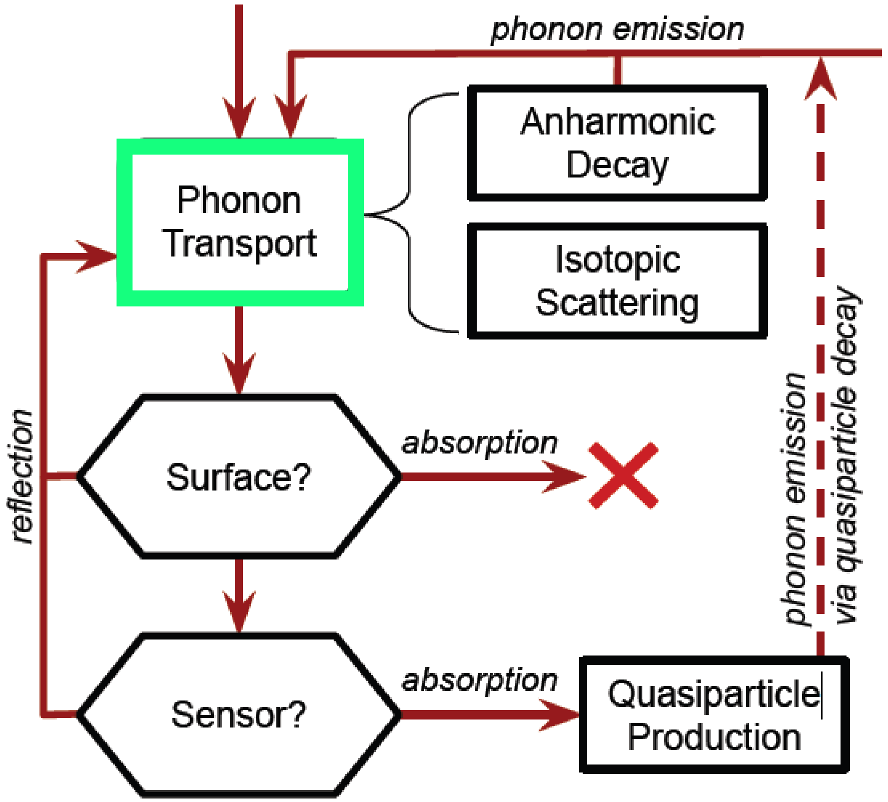


Figure 2: Comparison of phonon caustics predicted for a point source in a 1 cm thick Ge ⟨100⟩ crystal with corresponding results from G4CMP, showing positions of transverse phonon modes on the face opposite the point source. **Left:** Outline of phonon caustics in Ge ⟨100⟩ as predicted by Nothrop and Wolfe [34]. **Middle:** Caustics pattern as simulated using G4CMP for phonon transport in Ge ⟨100⟩, in good agreement with the theoretical prediction to the left. **Right:** Caustics pattern as simulated using G4CMP for phonon transport in a 1 cm thick Si ⟨100⟩ crystal (see also Ref. [16]).



Surface interactions

- Behavior of e/h and phonons at surfaces strongly depends on treatment, polish, fabrication recipe -> by default, particles that hit a surface are killed
- Can define simple optics-like surface interactions with explicit probabilities for absorption, reflection, transmission (currently not implemented), and specular-vs-diffuse reflection for phonons
- Phonons can also interact via Kaplan Quasiparticle model
  - Partitioning of energy into the superconducting film and back into substrate (as lower energy phonons) generated based on toy model of quasiparticle production and decay without actually simulating quasiparticles
- In progress effort to add true quasiparticle propagation

How to use G4CMP in your GEANT4 applications

- Install and setup geant4 10.7 as usual (not yet compatible with geant4 v11)
- Obtain g4cmp from github https://github.com/kelseymh/G4CMP
- Build and install with make or cmake, then source \`g4cmp_env.(c)sh\` to set required environment variables
- Add two lines to your application's cmake file:

```
find_package(G4CMP REQUIRED)
include(${G4CMP_USE_FILE})
```

- Add one line to your modular physics list:

```
RegisterPhysics(new G4CMPPhysics);
```

- Associate a crystal lattice to a physical volume:

```
G4LatticeManager* LM =  G4LatticeManager::GetLatticeManager();
LM->LoadLattice(physVol, latticeName /*"Ge" or "Si"*/);
```

What else is needed to get useful results?

- Specify mean free paths for charge trapping and impact ionization

G4CMP_ETRAPPING_MFP /g4cmp/eTrappingMFP [L] mm	Mean free path for electron trapping
G4CMP_HTRAPPING_MFP /g4cmp/hTrappingMFP [L] mm	Mean free path for charge hole trapping
G4CMP_EDTRAPION_MFP /g4cmp/eDTrapIonizationMFP [L] mm	MFP for electron-trap ionization by e^-
G4CMP_EATRAPION_MFP /g4cmp/eATrapIonizationMFP [L] mm	MFP for hole-trap ionization by e^-
G4CMP_HDTRAPION_MFP /g4cmp/hDTrapIonizationMFP [L] mm	MFP for electron-trap ionization by h^+
G4CMP_HATRAPION_MFP /g4cmp/hATrapIonizationMFP [L] mm	MFP for hole-trap ionization by h^+

- Specify electric field

G4CMP_VOLTAGE [V] /g4cmp/voltage [V] volt !=0:	Apply uniform +Z voltage
G4CMP_EPOT_FILE [F] /g4cmp/EPotFile [F] V=0	Read mesh field file "F"
G4CMP_EPOT_SCALE [F] /g4cmp/scaleEPot [F] V=0	Scale the potentials in EPotFile by factor F

- Define surfaces

```
auto* surfProp = new G4CMPSurfaceProperty(name,
                                           qAbsProb, // Prob. to absorb charge carrier
                                           qReflProb, // If not absorbed, prob to reflect
                                           eMinK, //Min wave number to absorb electron
                                           hMinK, //Min wave number to absorb hole
                                           pAbsProb, // Prob. to absorb phonon
                                           pReflProb, // If not absorbed, prob to reflect
                                           pSpecProb, //Prob. of specular reflection
                                           pMinK, //Min wave number to absorb phonon
                                           stype = dielectric_dielectric);
new G4CMPLogicalSkinSurface(name, logicalVolume, surfProp);
// or
new G4CMPLogicalBorderSurface(name, physVolume1, physVolume2, surfProp);

// to activate Kaplan quasiparticle physics
auto sensorProp = surfProp->GetPhononMaterialPropertiesTablePointer();
sensorProp->AddConstProperty("filmAbsorption", 0.20);    // True sensor area
sensorProp->AddConstProperty("filmThickness", 600.*nm);
sensorProp->AddConstProperty("gapEnergy", 173.715e-6*eV);
sensorProp->AddConstProperty("lowQPLimit", 3.);
sensorProp->AddConstProperty("phononLifetime", 242.*ps);
sensorProp->AddConstProperty("phononLifetimeSlope", 0.29);
sensorProp->AddConstProperty("vSound", 3.26*km/s);
sensorProp->AddConstProperty("subgapAbsorption", 0.1);

surfProp->SetPhononElectrode(new G4CMPPhononElectrode);
```

Improving computation speed

- Very many particles generated and tracked in typical G4CMP simulation
- Can specify downsampling factor for phonons and e/h for speedup
- Can also set max reflections before killing

Environment variable Macro command	Value/action
G4CMP_MAKE_PHONONS [R] /g4cmp/producePhonons [R]	Fraction of phonons from energy deposit
G4CMP_MAKE_CHARGES [R] /g4cmp/produceCharges [R]	Fraction of charge pairs from energy deposit
G4CMP_LUKE_SAMPLE [R] /g4cmp/sampleLuke [R]	Fraction of generated Luke phonons
G4CMP_MAX_LUKE [N] /g4cmp/maxLukePhonons [N]	Soft maximum Luke phonons per event
G4CMP_SAMPLE_ENERGY [E] /g4cmp/samplingEnergy [E] eV	Energy above which to down-sample
G4CMP_COMBINE_STEPLEN [L] /g4cmp/combiningStepLength [L] mm	Combine hits below step length

Environment variable Macro command	Value/action
G4CMP_EH_BOUNCES [N] /g4cmp/chargeBounces [N]	Maximum e^-/h^+ reflections
G4CMP_PHON_BOUNCES [N] /g4cmp/phononBounces [N]	Maximum phonon reflections
G4CMP_EMIN_PHONONS [E] /g4cmp/minEPhonons [E] eV	Minimum energy to track phonons
G4CMP_EMIN_CHARGES [E] /g4cmp/minECharges [E] eV	Minimum energy to track charges
G4CMP_MIN_STEP [S] /g4cmp/minimumStep [S] >0	Force minimum step SL0

How to add new lattices?

- Create a config.txt like the one for Si at right
- Parameter meanings documented in G4CMP Readme

```
# Crystal parameters
cubic 5.431 Ang          # (Lattice constant)
stiffness 1 1 165.6 GPa # C11, C12, C44
stiffness 1 2  63.9 GPa
stiffness 4 4  79.5 GPa
# Phonon parameters
dyn -42.9 -94.5 52.4 68.0 GPa
scat 2.43e-42 s3
decay 7.41e-56 s4
decayTT 0.74
# From S. Tamura et al., PRB44(7), 1991
LDOS  0.093
STDOS 0.531
FTDOS 0.376
Debye 15 THz             # Can also use temperature or energy
# Charge carrier parameters
bandgap 1.17 eV
pairEnergy 3.81 eV
fanoFactor 0.15
vsound 9000 m/s          # Longitudinal sound speed
vtrans 5400 m/s          # Transverse sound speed
l0_e 16.9e-6 m #16.9e-5 m # 8e-6 m #16.9e-6 m
l0_h 7.5e-5 m
#hole and electron masses taken from Robert's thesis
hmass 0.50               # per m(electron)
emass 0.91 0.19 0.19     # per m(electron)
valley   0  0  0 deg
valley   90 90 0 deg
valley   0 -90 -90 deg
# Intervalley scattering (matrix elements)
alpha 0.5 /eV
acDeform 6.6 eV
ivDeform 0.5e8 0.8e8 11e8 0.3e8 2e8 2e8 eV/cm           # Jacoboni & Reggiani
ivEnergy 12.0e-3 18.4e-3 61.8e-3 18.9e-3 47.2e-3 58.8e-3 eV
neutDens 1e11 /cm3
epsilon 11.68
# Intervalley scattering (Linear and Quadratic models)
ivModel Linear
ivLinRate0  1.5e6 Hz     # Fitted to Stanford test devices
ivLinRate1  1.5 Hz       # Fitted to Stanford test devices
ivLinPower  4.0          # Rate = ivLinRate0 + ivLinRate1 * E^ivLinPower
ivQuadRate  3.5e-20 Hz   # Fitted to Stanford test devices
ivQuadField 3395 V/m     # Fitted to Stanford test divices
ivQuadPower 7.47         # Rate = sqrt((E^2-QuadField^2)^ivPower)
```

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G4CMP User support

- Repository at https://github.com/kelseymh/G4CMP
- Historically development internal to SuperCDMS
- Hope to port internal issue tracker to github, and make use of github wikis, discussions, pull requests, etc.
- No official tag on GEANT4 forum, but relevant questions there usually get answered eventually

Thank you