

Texas A&M Activities for G4CMP ARO Grant



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Wade Lamberson, Dylan Monteiro, Nolan Tenpas

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Prof. David Toback
Principal Investigator



Michael Kelsey
Senior Research Scientist



Iman Atae-Langroudy
Graduate Student



Wade Lamberson
Graduate Student



Dylan Monteiro
Graduate Student



Nolan Tenpas
Graduate Student

Texas A&M Group

A&M has a large group with a long history of G4CMP leadership and development for both dark matter detectors and QIS

- Development and ongoing support of G4CMP by Kelsey supports both the SuperCDMS simulation effort and QIS device design and simulation

Four graduate students currently involved at various levels working on their degrees under the supervision of Toback

- Ataee-Lagroundy is completing his Ph.D. thesis soon
- Lamberson is completing his ramp-up as a full-time expert

Outline of A&M Activities

Overall G4CMP management, releases

Consultation for QIS community members

Migration to Geant4 11

Charge transport and surface interactions

Phonon surface modes (creation and pseudo-transport)

Theoretical calculation of phonon normal modes

Dominant G4CMP issues for decoherence

Overall G4CMP Management, Releases

Kelsey (Senior Research Scientist)

- JIRA ticketing system
both bugs and new features
- Coding guidelines (Yamaoka, LPS)
- Code reviews before integration
- Single line of development
feature → develop → main
- Frequent (1-2 month) releases

Software reviews usually include
experienced G4CMP developers

The screenshot displays the SLAC JIRA interface. The top navigation bar includes links for Dashboards, Projects, Issues, Boards, Plans, Assets, and a Create button. A search bar is located on the right. The main content area shows an 'Open issues' list on the left with a 'Switch filter' dropdown. The selected issue, 'G4CMP-511: Create parallel Lambertian reflection code for charges', is displayed in the center. The issue details include a description, type (Sub-task), priority (Major), and labels (None). The right sidebar shows the issue's status (In Progress), assignee (Lamberson, Wade), reporter (Michael Kelsey), and a 'Stop watching this issue' button. Below the issue details, there is a 'Releases' section with a 'Tags' tab. The 'Tags' tab lists several releases, including G4CMP-522, g4cmp-V09-09-02, G4CMP-533, G4CMP-527, and g4cmp-V09-09-01, each with a download link for a tar.gz file.

Consultation for QIS Community Members

Kelsey

We provide guidance and suggestions on how to use G4CMP for several QIS investigators, and will continue to do so

- Spin-qubit systems, with charge transport (Lutz, Sandia)
- Modeling of MKID sensors (**Kurinsky, Dang**, SLAC)
- Phonon propagation across thin films (Hebenstiel, IU)

As a member of the Geant4 Collaboration, Kelsey has also acted as a liaison with Geant4 experts to improve overall simulation performance, migrate to G4 11, etc.

Migration to Geant4 Version 11

Inman (PNNL), Johnson (LLNL), **Kelsey**, Linehan (NW), Zatschler (SNOLAB)

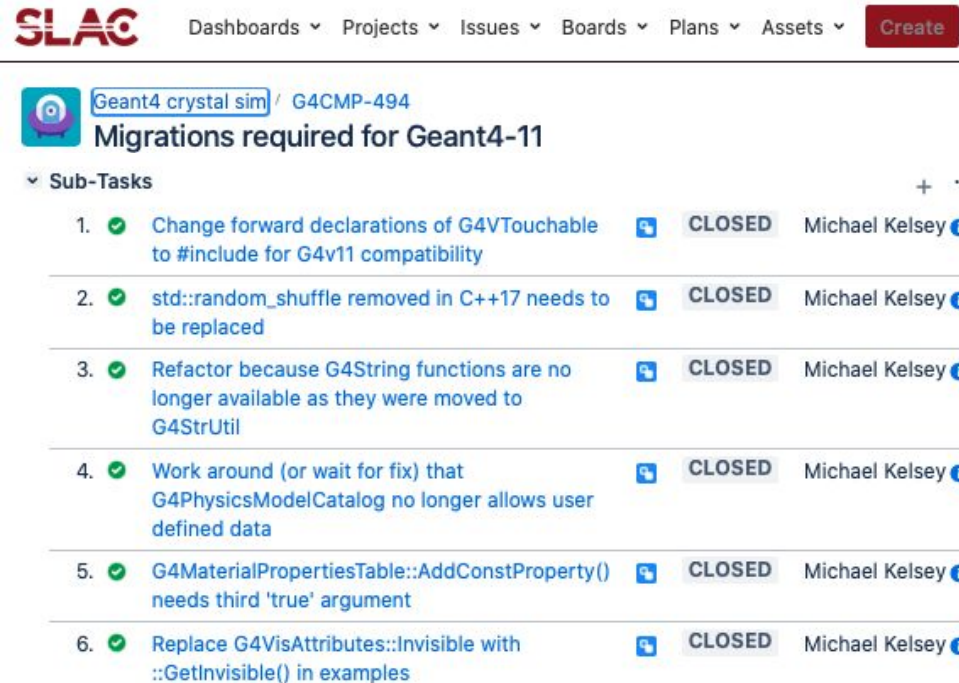
G4CMP compatible with Geant4 10.07.p04, ~4 years past end of life

Support for Geant4 11.3.2 (11.4.0) strongly desired by QIS community

Required nine modification to code (tracked with JIRA tickets)

- G4String/G4StrUtil, G4VTouchable, MPT, std::shuffle, ParticleChange, G4VisAttributes
- G4PhysicsModelCatalog apparent blocker being resolved with patches on Geant4 side
- Additional issues identified and resolved with runtime testing

All modifications implemented to be compatible with both G4 v10 and v11



The screenshot shows a JIRA project page for 'Geant4 crystal sim' with the issue 'G4CMP-494' titled 'Migrations required for Geant4-11'. The page lists 6 sub-tasks, all of which are marked as 'CLOSED' and assigned to 'Michael Kelsey'.

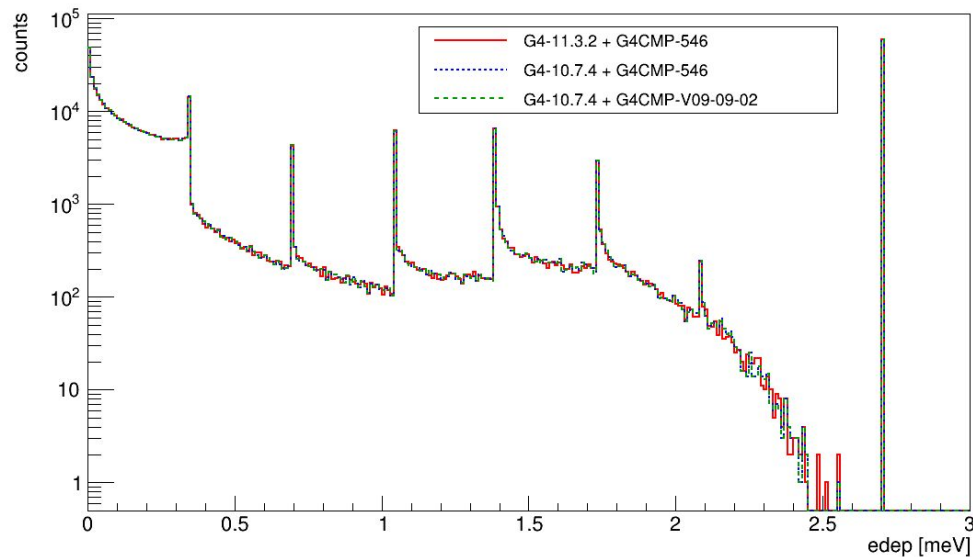
Sub-Task	Status	Assignee
1. Change forward declarations of G4VTouchable to #include for G4v11 compatibility	CLOSED	Michael Kelsey
2. std::random_shuffle removed in C++17 needs to be replaced	CLOSED	Michael Kelsey
3. Refactor because G4String functions are no longer available as they were moved to G4StrUtil	CLOSED	Michael Kelsey
4. Work around (or wait for fix) that G4PhysicsModelCatalog no longer allows user defined data	CLOSED	Michael Kelsey
5. G4MaterialPropertiesTable::AddConstProperty() needs third 'true' argument	CLOSED	Michael Kelsey
6. Replace G4VisAttributes::Invisible with ::GetInvisible() in examples	CLOSED	Michael Kelsey

Migration to Geant4 Version 11

Tested using G4CMP Phonon example

- Last release tag with 10.07.p04
- Migration branch with 10.07.p04
- Migration branch with 11.3.2

Results statistically identical (G4 v11 has slightly different random sequence)



Histogram shows energy absorbed by aluminum QET fins on surface of detector: spikes at 2Δ , 4Δ , 6Δ , 8Δ , 10Δ , 12Δ . Primary 2.8 meV phonons and phonon $< 2\Delta$ can be absorbed directly by tungsten TES

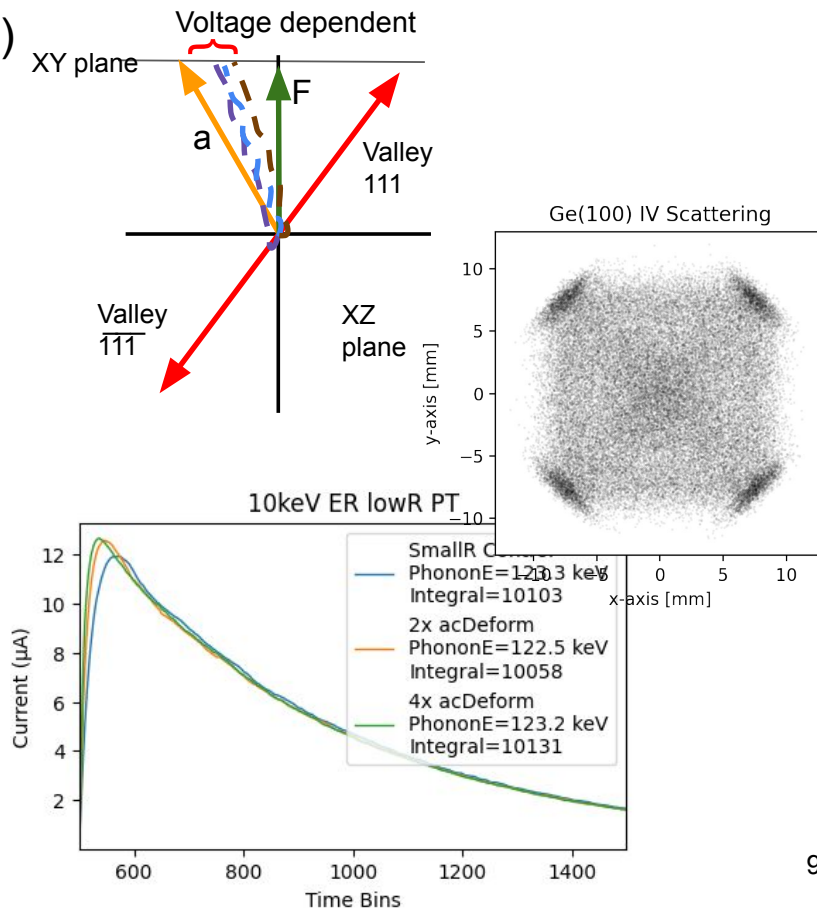
Charge Transport Intervalley Tuning

Ataee-Langroudy, Monteiro (Graduate Students)

Ataee completed a major revision of physics-based electron transport and scattering in 2024

- Completing his thesis in next month
- Will publish as a short paper after

Monteiro is validating and tuning physics-based intervalley scattering model (**Michaud**/SNOLAB)



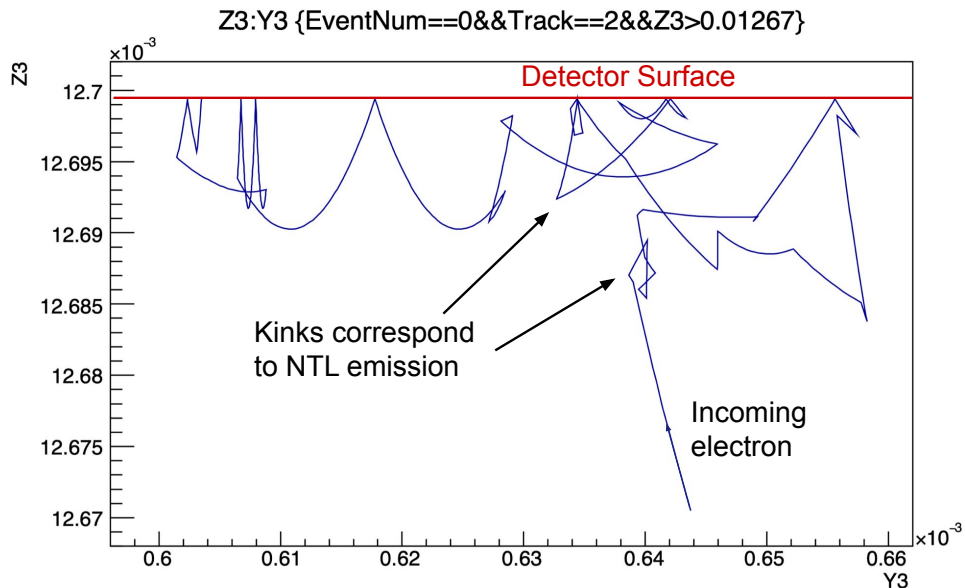
Charge Carrier Surface Interactions

Kelsey, Lamberson (Graduate Student)

Enable charges to reflect off surfaces

Electron reflection has non-trivial effects due to valleys and anisotropic mass tensor

Lamberson working on improving model for charge reflection under these conditions.



Upcoming: incorporate charge recombination in crystal bulk, when charge momentum drops below threshold for NTL emission (complicated with E-field!)

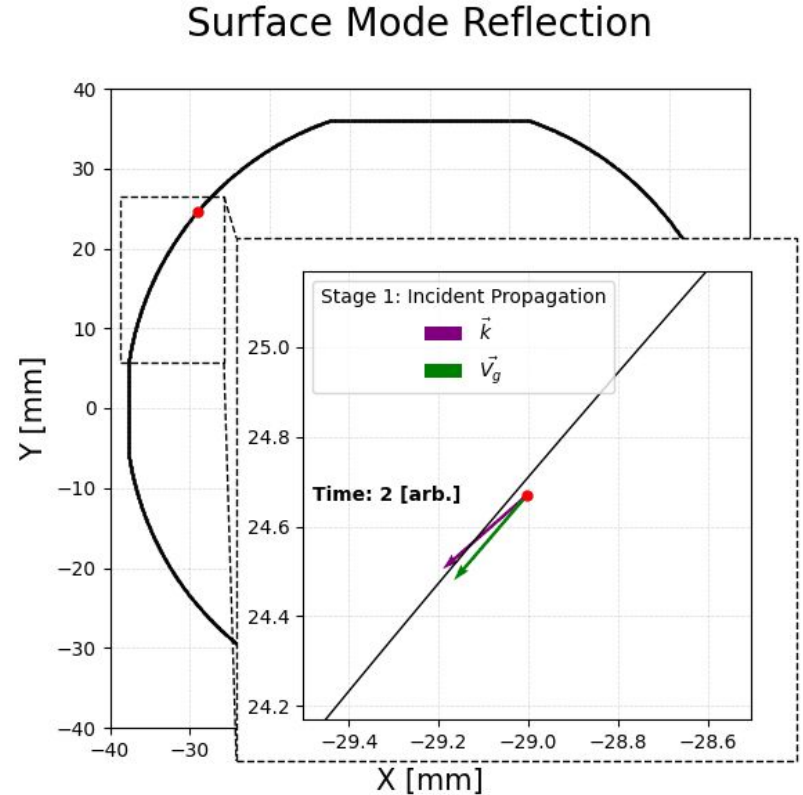
Phonon Surface Modes

Lamberson, Tenpas (Graduate Student)

Phonons reflection at polished surfaces can fail

Dispersion relation may direct group velocity (V_g , **green**) out of crystal, even if reflected wave vector (k , **purple**) is inward

Developed and deployed a comprehensive framework to handle this, emulating surface mode as displacement of position to where V_g is inward



Note: All vectors have been scaled equally for visual effect

Phonon Surface Splitting

Lamberson, Tenpas

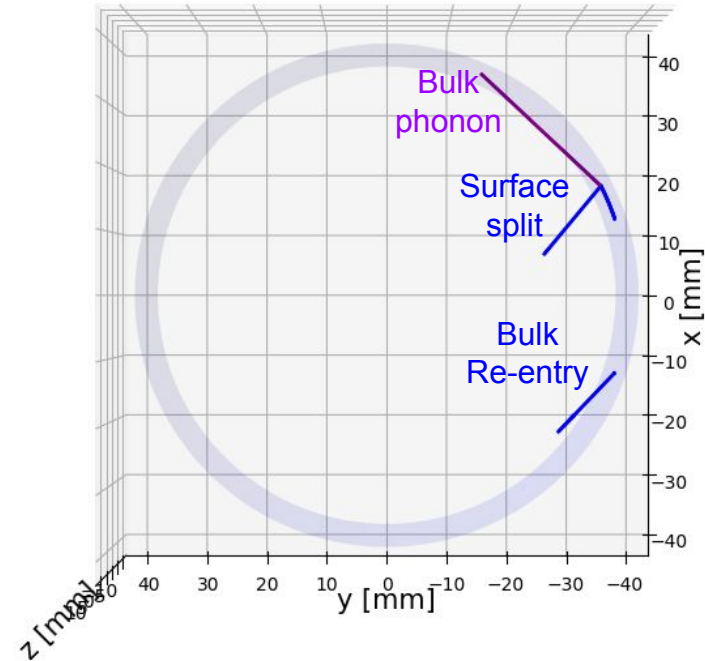
Converting phonons to and from surface modes is not physically correct, should be $B \rightarrow B R$

Surface mode energy would be $\mathcal{O}(\text{neV})$ vs. $\mathcal{O}(\text{meV})$ for bulk phonons: not worth implementing?

Considering computing "lost" energy as part of diffuse scattering

Would make some event-level sanity checks (e.g.,

E_{expected} vs. $E_{\text{collected}}$) more difficult



CDMS-style crystal viewed from above

Calculation of Phonon Normal Modes

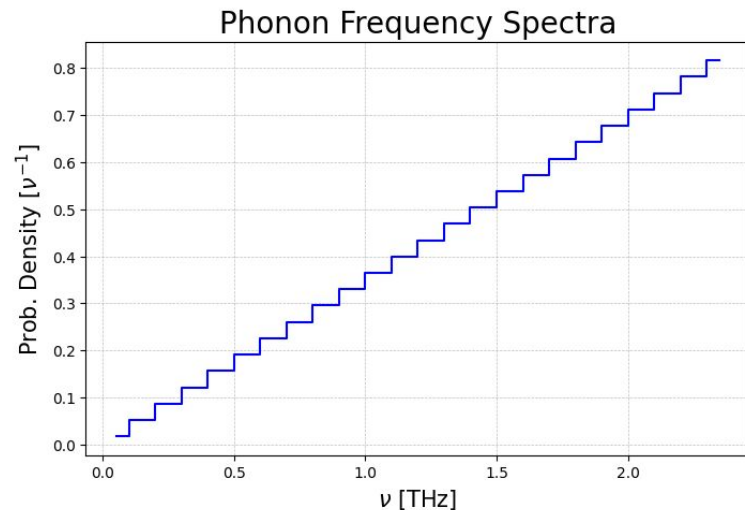
Tenpas

Working with Prof. Valery Pokrovsky (A&M) to complete an analytical 3D calculation of phonon normal modes in a cylindrical detector (CDMS-style)

Includes the full stiffness matrix formalism and phonon dispersion relations to obtain energy spectra and limits

This work (paper in preparation) significantly improves our grounding in theoretical dynamics of phonons in crystals

Gives us insight into physically motivated boundary conditions, distribution functions, and spectra (PDFs) for G4CMP processes



Dominant Issues for Decoherence

Lamberson

Identifying the dominant issues related to qubit decoherence effects which should be simulated or simulatable with G4CMP

- Time-Dependent Quasiparticle Diffusion, Recombination, and Trapping in Superconducting Films (**Linehan**, G4CMP-219)
- Improved Modeling of QP Generation at Substrate-Superconductor Interfaces (Golwala/Caltech, G4CMP-331, G4CMP-332)
- Gap Engineering and Variable Superconducting Properties, Additional Materials (**Linehan**)
- Non-Ionizing Phonon Sources from Mechanical Stress and Thermal Contraction (CDMS HVeV and others)
- Spatiotemporal Correlations and Large-Scale Device Geometries in QIS Arrays (**Linehan**, G4CMP-219 and RISQ Tutorial)

This study expected to be **Lamberson's** Master's topic, and may become his Ph.D. topic

Summary and Upcoming Work

G4CMP is fully functional and in use by an increasing number of groups

Contributions are well organized and tracked from request/report to deployment

Improvements to the physics of phonon and charge transport continue incrementally, along with significant new features (**Kelsey**, **Lamberson**, **Monteiro**, **Tenpas**)

Expect **Ataee**'s thesis on electron transport to be completed in next month

In the next few months, expect to complete work on charge reflection (**Lamberson**), evaluate effect on phonon arrival time distributions

Coordinating final integration of **Linehan**'s QP tracking and RISQ Tutorial

Develop **Lamberson**'s work on decoherence into a more concrete plan, identifying which issues are already in process, and which we should take on ourselves