STSM REPORT

COST STSM Reference Number: STSM-BM1205-160514-044692

STSM Grantee: Mr Andrew Grier (PhD researcher)

STSM title: Development and optimisation of MIR and THz QCL modelling software

Home Institution: School of Electronic and Electrical Engineering, University of Leeds, UK

Host Institution: Tallinn University of Technology, Estonia

Host: Dr Andres Udal

STSM period: 16/05/2014 – 24/05/2014

STSM purpose: Consolidate and expand collaborative efforts between groups to develop and optimise software used to model quantum cascade lasers for use in imaging

Description of the work carried out during the STSM:

The University of Leeds and Tallinn University of Technology have previously collaborated on the development of quantum cascade laser (QCL) modelling software and this STSM facilitated the consolidation and discussion of independent efforts. Furthermore, we discussed strategies for the optimisation of our software so that simulations are faster and converge reliably. The motivation of this is to allow the use of the software as a QCL design tool for future design innovations in the terahertz (THz) and mid-infrared (MIR) regions of the electromagnetic spectrum.

QCL models are often used to model current and gain over a range of lattice temperatures and applied biases. Since these models typically use iterative techniques to find self consistent input parameter values, we focussed on implementing the reuse of input parameters such as electron temperature and subband populations from previous data points for faster convergence. This time-saving will be critical for genetic optimisation algorithms, where several thousand device variations are required.

Additionally, the grantee gave two talks at the host institution that were useful in conveying the motivation for THz and MIR imaging at Leeds as well as discussing current research challenges.

Research and design of modern quantum electronics devices at Leeds University
MSc lecture 20th May 2014

Research and design of quantum optoelectronic devices for terahertz and infrared sensor technologies
Presentation 22nd May 2014

Description of the main results obtained:

Strengthened relationship between researchers at separate groups. Lectures and seminars given by the grantee presented the merits of different modelling techniques such as the rate equation, density matrix and Non-Equilibrium Green's functions. Academic presentation included an extended presentation on density matrix modelling applied to both AlGaAs and AlGaN QCLs.

The reuse of subband electron temperatures to obtain kinetic balance between the lattice and subband populations resulted in a runtime improvement of ~ 25% for applied bias sweeps. This was achieved by using previous values as the starting point for the new interval search in the full self-consistent simulation shown in Figure 1.

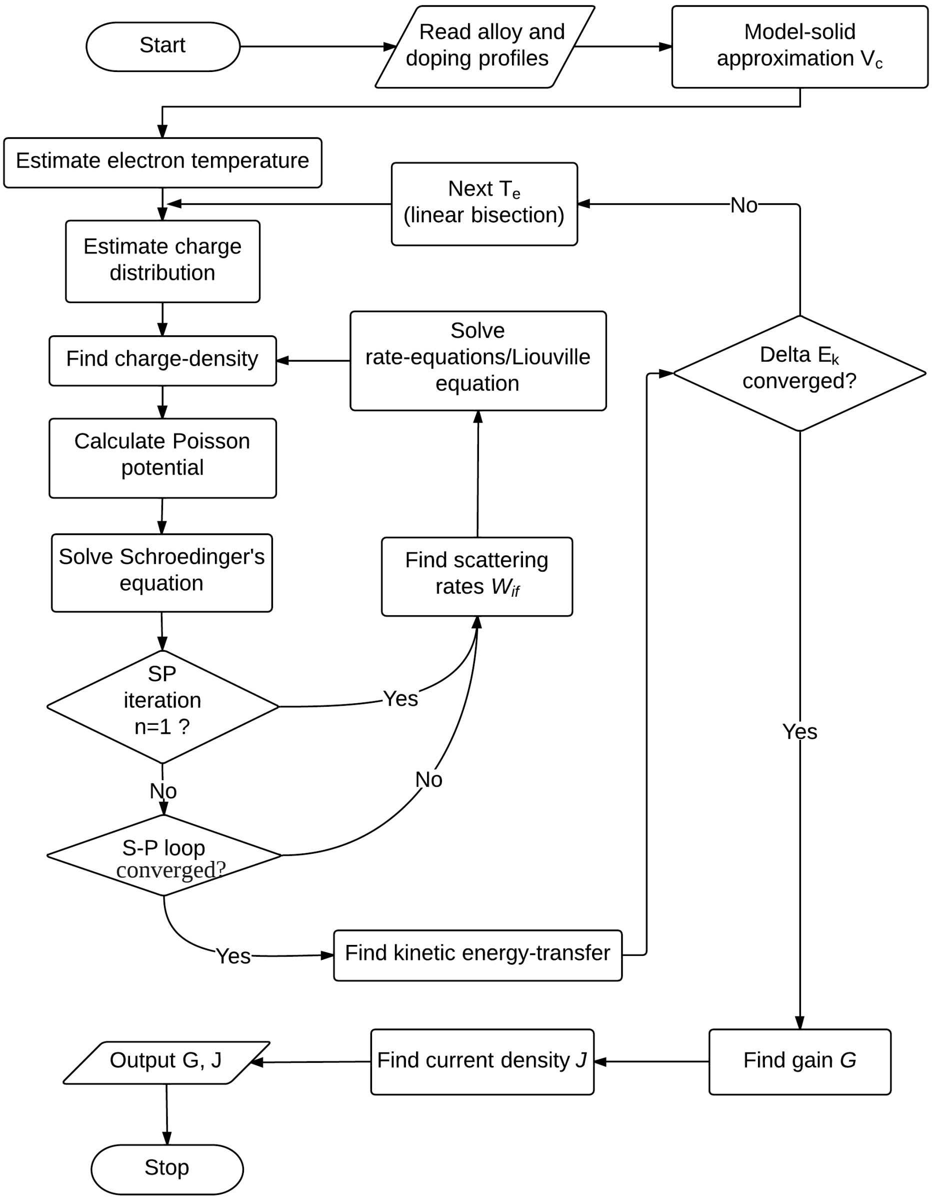

Figure 1: Flowchart for a QCL simulation at a single field or lattice temperature point

When applied to a QCL structure such as that shown in Figure 2, this model provides gain and current data which has good experimental agreement. Figure 2 also shows the variation of the subband electron temperature that results in kinetic energy balance with lattice temperature. By optimising the linear bisection interval range, convergence is achieved faster.

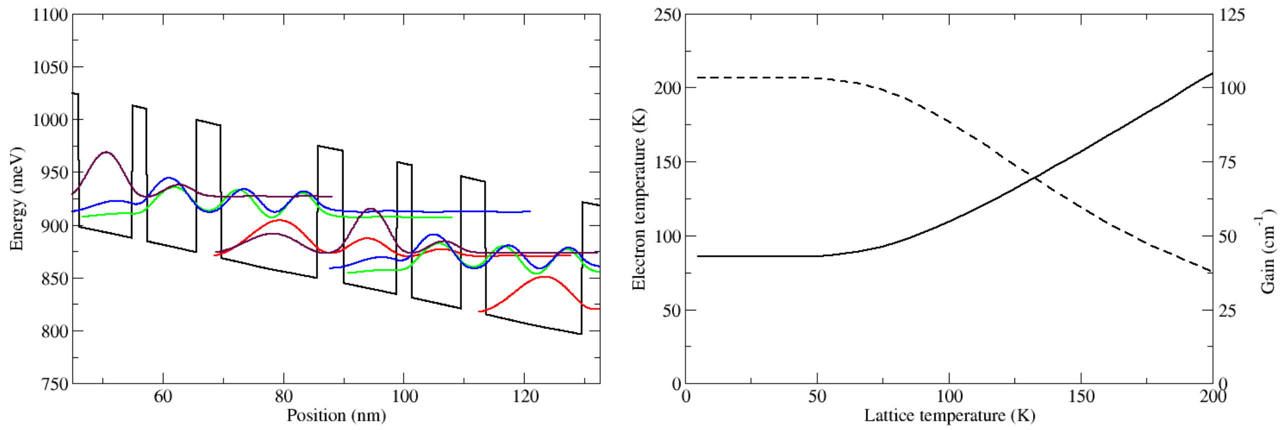

Figure 2: a) Bandstructure and wavefunction plot for the current high temperature record design [1] b) Electron temperature and unsaturated gain versus lattice temperature for this structure

The number of Schrödinger-Poisson loops needed for a self-consistent solution varies between devices significantly depending on doping and the number of states in a period. Therefore initial work on the development of an intelligent convergence check was completed. Eventually, this will ensure that software users will have a converged solution which is critical for accurate gain and current output. Additionally, a PhD student at Tallinn has implemented the reuse of subband populations in the self-consistent Schrödinger-Poisson solution and this approach was also discussed for future collaborative work.

Mutual benefits for the Home and Host institutions:

Collaboration with the group in Tallinn University of Technology was useful and stimulating, with many aspects of QCL modelling discussed between the visitor and host. By discussing challenges encountered and the work completed to date, the group at Leeds has a better understanding of possible optimisation areas. The group in Tallinn will benefit from the discussion of the density matrix approach for QCL modelling which has several advantages over the rate equation approach. Perhaps most significantly, comparison of the output of QCL models which have been developed independently will allow objective verification of results in the future.

Future collaboration with the Host institution (if applicable):

Several areas for future collaboration between groups were conceived. In the short-term it is desirable to complete the optimisation and testing of the modelling code so that it is a fast, reliable foundation for future work. In the long-term we aim to develop the inclusion of photon density within the laser cavity which has potential applications in image modelling as well as allowing predictive modelling of output power. This could potentially be applied to and compared with experimentally characterised devices in a future publication.

References

[1] S. Fathololoumi et al., *Terahertz quantum cascade lasers operating up to ~ 200 K with optimized oscillator strength and improved injection tunneling* Optics express **20**, 3866-3876 (2012).