Converged Simulations of a TeraHertz Oscillator

A collaboration between researchers at NC State and Sandia's CCIM center 1400 has led to a unique computational capability for modeling a Resonant Tunneling Diode (RTD). An RTD is a nanoscale electronic device (see Fig. 1) that is believed to autonomously oscillate under certain conditions by quantum tunneling effects. The TeraHertz frequency of the oscillations makes the RTD of interest for numerous applications, including medical imaging, sensing, chemical analysis, and applications of interest to DoD.

The Wigner-Poisson equations govern the behavior of the electrons in the device, where even a one-dimensional geometric model results in a two-dimensional calculation over space and momentum. The equations have both integral and differential components that lead to a dense interaction matrix between all nodes. A typical solution of the model is an entire current-voltage (I-V) curve, which can include hysteresis effects and regions of oscillations. Before this collaboration, the state-of-the-art was a 6 Thousand node model where oscillatory states were observed by long time integration.

Under a CSRI-funded collaboration, the Wigner-Poisson code was interfaced to the Trilinos solver framework to make use of the continuation, bifurcation, eigensolver, linear solver, nonlinear solver, and parallel data structure packages. A parallelization strategy was devised and implemented (Fig. 2) to increase the problem sizes that could be tackled, and an eigensolver was used to detect the onset of oscillations *via* a Hopf bifurcation.

Parallel computations on 48 processors of the ICC cluster were sufficient to perform mesh refinement studies for the entire I-V curve up to 2 Million unknowns, and demonstrate mesh convergence of the model for the first time. An analysis found that the algorithm was 95% parallel and 5% sequential. This scalability is adequate for this model, (with ~60% parallel efficiency on 16 processors) but shows that the algorithm would not scale well if convergence required the resources of RedStorm.

The collaboration has led to 3 journal publications, and has spawned a new collaboration under NECIS funding.

Contact: Andy Salinger (Org. 1416) 505-845-3523, with Prof. C.T. Kelley and Matthew Lasater of NC State.

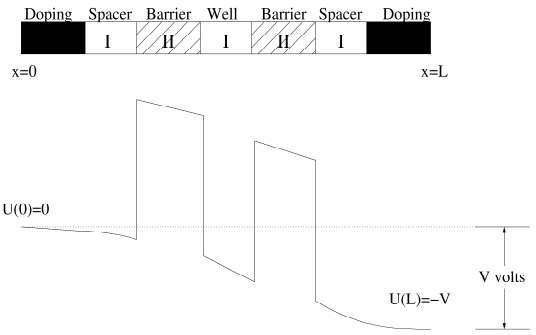

Fig 1: Schematic of Resonant Tunneling Diode

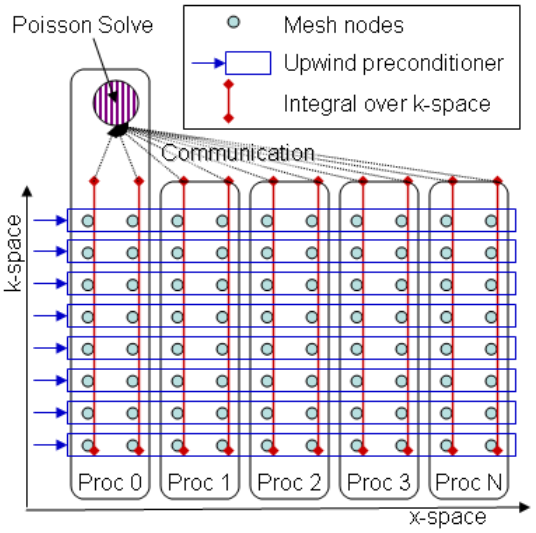

Fig 2: Parallel Computation Strategy

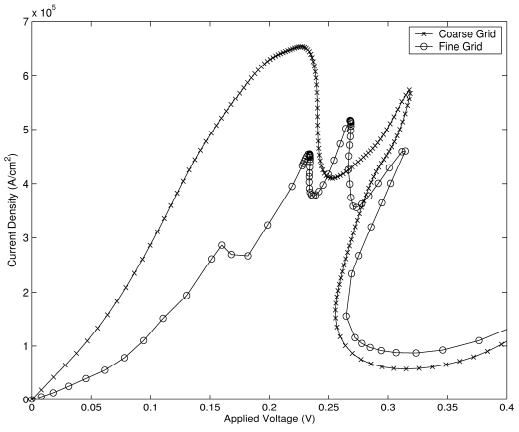

Fig 3: Change in Current-Voltage diagrams with mesh refinement from 6 Thousand nodes to a converged solution of 2 Million nodes.