Solution of the Wigner-Poisson Equations for RTDs

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DCABES 2004

Wuhan, China, September 2004

Supported by ARO, NSF.

Outline

- Wigner-Poisson Equation
  - Cost of evaluation.
  - Parameter tracking.
- Parallel Computation
  - SANDIA nonlinear solver tools: NOX and LOCA
  - TRILINOS infracstucture
- Future work
- Conclusions

Wigner-Poisson Equation for $f(t,x,k)$

$$\frac{\partial f}{\partial t} = -\frac{hk}{2\pi m^*}\frac{\partial f}{\partial x} - V(f) + \left.\frac{\partial f}{\partial t}\right|_{coll},$$

where

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{1}{\tau}\left[\frac{f_0(x,k)}{\int dk f_0(x,k)}\int dk f(x,k) - f(x,k)\right].$$

h: Planck's constant; m^*: effective mass of electron

τ: relaxation time; f_0: equilibrium distribution

Potential Energy Term

$$V(f)(x,k) = \frac{1}{h}\int dk' f(x,k') \int dy[U(x+y)-U(x-y)]sin[2y(k-k')].$$

where

$$U(x) = u(x) + \Delta_c(x)$$

$$u_{xx}(x) = \frac{q^2}{\epsilon}[N_d(x) - n(x)], u(0) = 0, u(L) = -V_{bias}$$

$$n(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} f(x,k)$$

Δ_c: potential barriers; N_d: doping profile

q: electron charge; ϵ: dielectric permittivity

Computational Costs

Discretize with n_x points in x and n_k in k. Costs:

- $n(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} f(x,k)k$: $O(n_x n_k)$.
- $\frac{d^2}{dx^2}u(x) = \frac{q^2}{\epsilon}[N_d(x) - n(x)]$: $O(n_x)$.
- $\frac{\partial f}{\partial t}\Big|_{coll} = \frac{1}{\tau}\left[\frac{f_0(x,k)}{\int dk f_0(x,k)}\int dk f(x,k) - f(x,k)\right]$: $O(n_x n_k)$.

$$V(f) = \frac{1}{h}\int dk' f(x,k')\int dy[U(x+y) - U(x-y)]sin[2y(k-k')].$$

direct evaluation: $O(n_x^2 n_k^2)$.

Use FFT and be clever to get $O(n_x n_k(\log n_x + \log n_k))$.

Parameter-dependence Study

Solution dynamics depend on boundary conditions for

$$\frac{d^2}{dx^2}u(x) = \frac{q^2}{\epsilon}[N_d(x) - n(x)]$$

which are

$$u(0) = 0; u(L) = -V_{bias}.$$

Objectives:

- Explain prior numerical observations of hysteresis.
- Find values of V_{bias} for which f is periodic in time.

Path Following

$F : X \times [a, b]$, F smooth, X a Banach space.
Objectives:

- Solve $F(u, \lambda) = 0$ for $\lambda \in [a, b]$
- Understand $u_t = F(u, \lambda)$ by looking at spectrum of F_u

Obvious approach:

Set $\lambda = a$, solve $F(u, \lambda) = 0$ with
Newton-(MG, GMRES, . . .) to obtain $u_0 = u(\lambda)$.
while $\lambda < b$ **do**
  Set $\lambda = \lambda + d\lambda$.
  Solve $F(u, \lambda) = 0$ with u_0 as the initial iterate.
  $u_0 \leftarrow u(\lambda)$
end while

What's the problem?

- Multiple solutions, hysteresis
- Changes in dynamic stability
- No solutions

A fix: Pseudo-arclength continuation.
Set $x = (u, \lambda)$ and solve $G(x, s) = 0$, where, for example

$$G(x,s) = \begin{pmatrix} F \\ N \end{pmatrix} = \begin{pmatrix} F(u(s), \lambda(s)) \\ \dot{u}^T(u - u_0) + \dot{\lambda}^T(\lambda - \lambda_0) - (s - s_0) \end{pmatrix}.$$

s is an artificial "arclength" parameter.
u_0 and λ_0 are from the previous step.

$\dot{u} \approx du/ds$ and $\dot{\lambda} \approx d\lambda/ds$.

Simple Folds

We follow solution paths $\{x(s)\}$ to better understand $u_t = F(u, \lambda)$.
Assume that F is smooth and

- G_x is nonsingular (not always true) So implicit function theorem holds in s.

We are assuming that there is no true bifurcation and that any singularity in λ is at worst a simple fold.

- dimKer$(F_u) = 1$
- $F_\lambda \notin$ Ran(F_u)

Hopf Bifurcations

We also look for Hopf Bifurcation,

- A complex conjugate pair of eigenvalues of F_u cross the imaginary axis from the left.
- Leads to periodic dynamics for $u_t = F(u, \lambda)$.

Arclength Continuation Algorithm

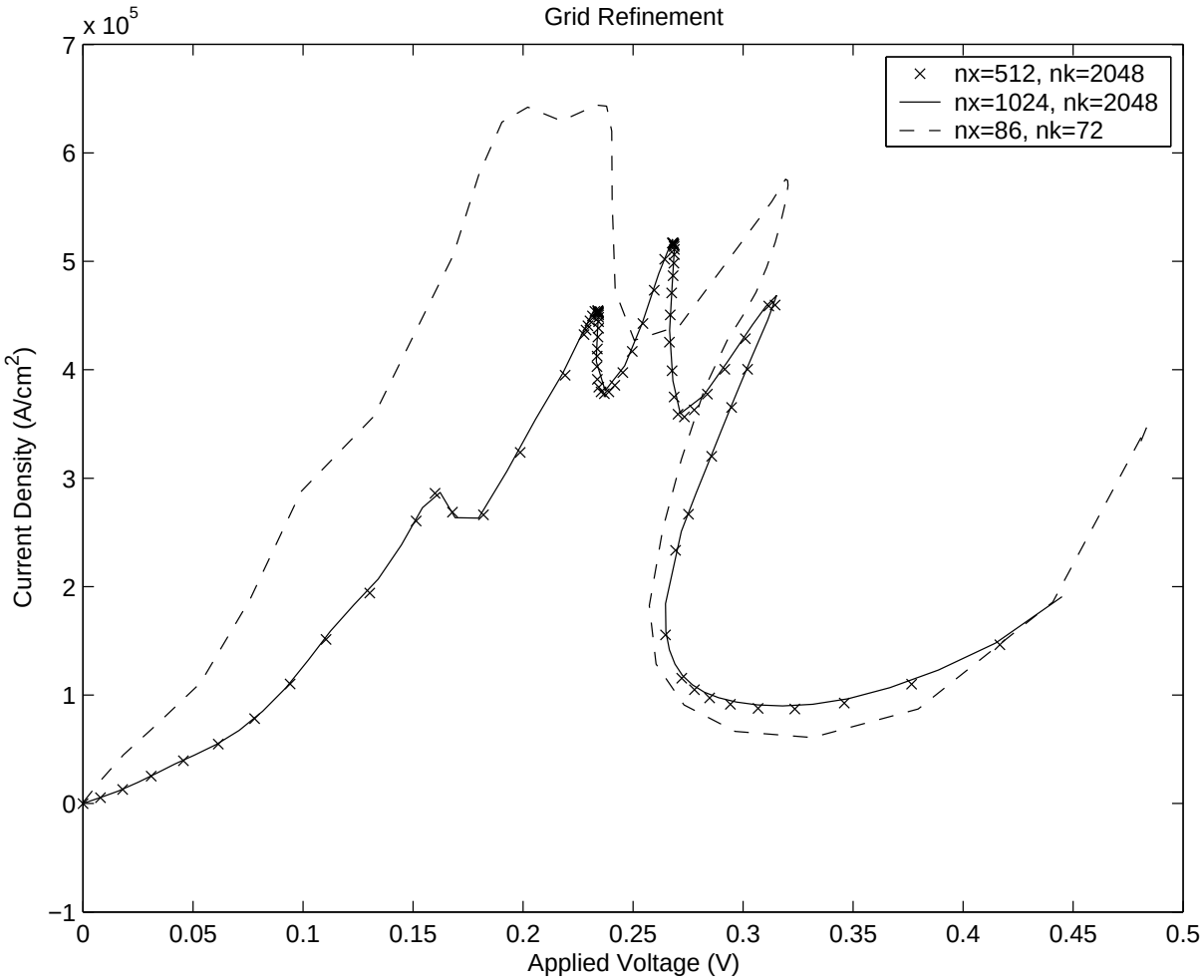
Set $\lambda = a$, $s = 0$ solve $F(u, \lambda) = 0$ with Newton-(MG, GMRES, . . .) to obtain u_0.
Estimate ds, $\dot{u}$, $\dot{\lambda}$.
while $s < s_{max}$ **do**
  $s \leftarrow s + ds$.
  Solve $G(x, s) = 0$ with u_0 as the initial iterate.
  Examine F_u or G_x for folds and bifurcations.
  $x_0 \leftarrow x$
  Update ds, $\dot{u}$, $\dot{\lambda}$.
end while

Path following for Wigner Poisson Eq

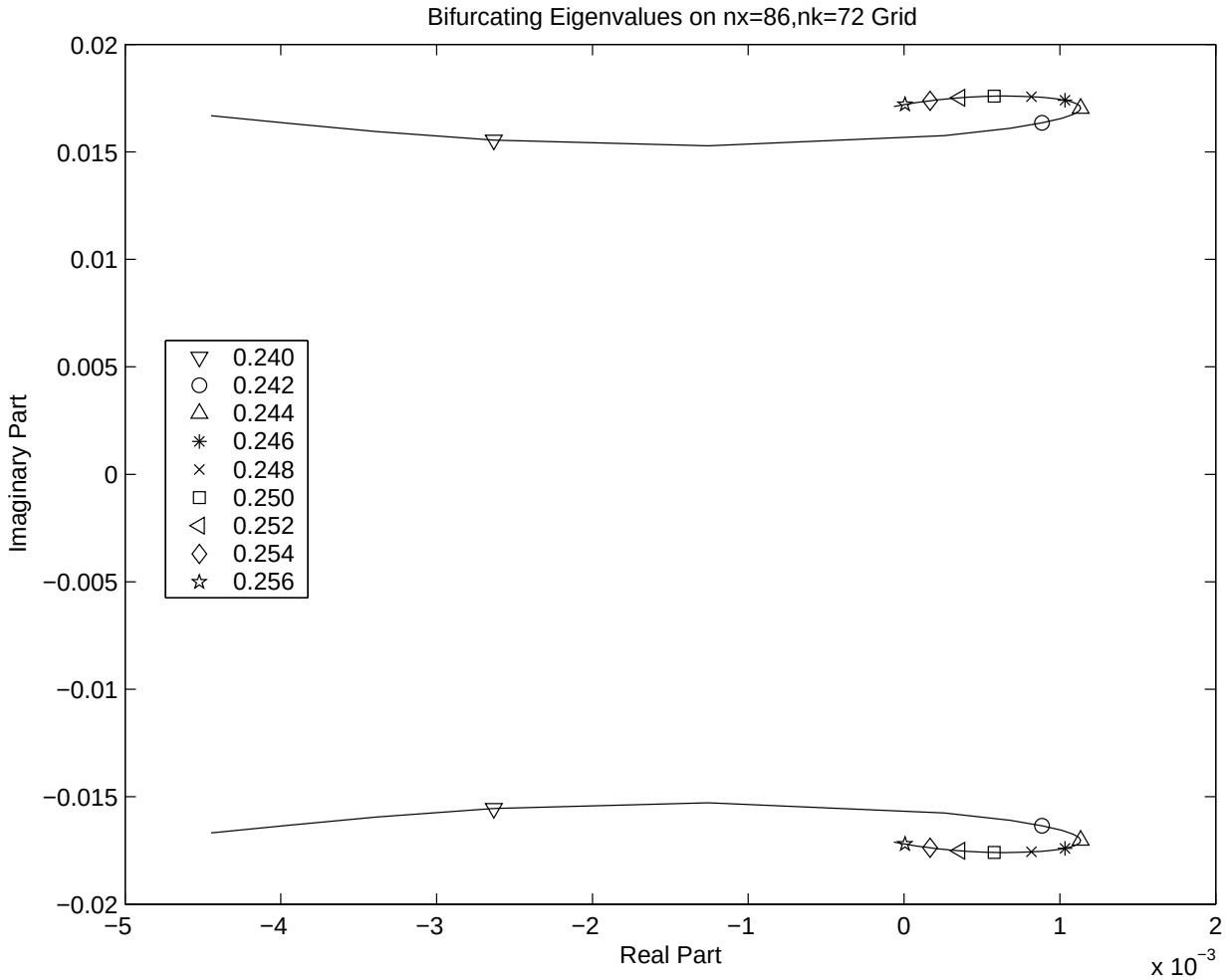
- Use LOCA (Salinger-Phipps)
  NOX, AztecOO, Anasazi, Epetra
- Precondition with inverse of spatial differential operator
- Uniformly bounded, not quite compact
- Folds, hysteresis, Hopf bifurcation
- Figure: Current density $j(x)$ at $x = L$ vs V_{bias}

$$j(x) = \frac{h}{2\pi m^*} \int k f(x,k) dk$$

Latest LOCA results; new physics



Hopf bifurcation on coarse grid



LOCA

- Part of Trilinos - Sandia's parallel solver project
- Makes use of several other parts of Trilinos:
  - NOX : Nonlinear solver
    Preconditioned Newton-Krylov
  - AztecOO : Preconditioned Krylov linear solvers
  - Anasazi : Eigensolver
  - Epetra : Data Structure

Parallelism

- Each processor has a block in space, all of momentum FFT convolution in k; BLAS3 for convolution in x.
- Epetra data structures used in simulator + all solvers
- Computations on various LINUX clusters.

Parallel Efficiency

Continuation with $n_x = 688$, $n_k = 576$

# Procs.	Linear Solve Time (s)	Speedup	Efficiency (%)
1	431.21	—	—
2	263.69	1.64	82.0
4	115.71	3.73	93.3
8	75.23	5.73	71.6
16	45.38	9.50	59.4

Scalability

Scalability of Parallel Simulator

N_x	N_k	# Procs.	Avg. F Eval Time (s)
172	144	1	0.1209
344	288	4	0.2814
688	576	16	0.5505

Tricky: not the same problem at all grids.

Bottom line: 40% scalar code.

Conclusions

- Parametric study of Wigner-Poisson Equation
- Finding new physics
- Scalable Preconditioner
  Still too much scalar code
- Hysteresis understood
- Hopf understood on coarse grids
  working on eigensolver for fine grids