

# Notes for Stan, June 6, 2003

## 1 A brief synopsis of Monte Carlo codes to synchronize notation

I am not so familiar with Shaikh's code. So, for the details you will to ask him or refer to his thesis. The following is just a simple synopsis of how these things work.

Generally, Monte Carlo methods approximate a positive density function  $f(x, p, t)$  by a superposition of  $\delta$ - functions, i.e.

$$f(x, p, t) \approx \sum_{n=1}^N \delta(x - x^n(t)) \delta(p - p^n(t))$$

(I usually write things in terms of momentum, so  $p = \hbar k$  holds, while Shaikh uses wave vectors  $k$ . This is just a simple matter of notation. Also superindices are used for particles while subindices are used for components of vectors.) Now the issue is how to update the positions  $x^n$  and momenta  $p^n$ . Generally speaking this is a two stage process.

So, given the  $x^n(t)$  and  $p^n(t)$  for  $n = 1, \dots, N$

Step 1:

Move the particles according to free flight, i.e. according to Newton's second law  $F = ma$ . This means

$$\frac{d^2}{dt^2} x^n(t) = a = \frac{F}{m} = -\frac{e}{m} \nabla_x V(x^n, t)$$

So the force  $F$  is given by  $-e \nabla_x V$ , where  $e$  is the charge of the electron and  $m$  is the mass of the electron. Defining the velocity  $\frac{d}{dt} x^n(t) = \frac{p^n(m)}{m}$ , this gives

$$\frac{d}{dt} x^n(t) = \frac{p^n}{m}, \quad \frac{d}{dt} p^n(t) = -e \nabla_x V(x^n, t) \quad (1)$$

Now, the above holds only in a vacuum. Half of the complication of Monte Carlo for semi-conductors arises from the fact that the electron moves in a crystal. In this case the relation between velocity ( $\frac{d}{dt} x^n(t)$ ) and momentum ( $p$ ) is a bit more complicated and (1) is replaced by

$$\frac{d}{dt} x^n(t) = v(p^n) = \nabla \varepsilon(p^n), \quad \frac{d}{dt} p^n(t) = -e \nabla_x V(x^n, t) \quad (2)$$

The function  $\varepsilon(p)$ , whose gradient gives the velocity, is called the band diagram, which is computed once for a given material. In a vacuum  $\varepsilon(p) = \frac{|p|^2}{2m}$  holds, and (2) reduces to (1). Now, depending how realistic you want to be, you either have a tabulated band energy  $\varepsilon$ ,

computed from a Schrödinger equation calculation (this is called 'full band Monte Carlo'). or various approximations for  $\varepsilon(p)$ . My understanding is that Shaikh uses the Herring - Vogt model. (I am sure that's somewhere in his thesis). Anyway, (2) is now implemented as

$$x^n(t + \Delta t) = x^n(t) + \Delta t \nabla \varepsilon(p^n(t)), \quad p^{n0}(t + \Delta t) = p^n(t) - \Delta t e \nabla_x V(x^n, t) \quad (3)$$

Note that we have written  $p^{n0}(t + \Delta t)$  instead of  $p^n(t + \Delta t)$ , since we are changing  $p^n$  once more in the second stage of the process.

Step 2:

This step involves the scattering process. In scattering  $p^n$  changes randomly according to a certain probability given by the scattering rate  $S(p, q)$ . I.e., in standard probability notation, we chose a new momentum vector  $p^n$  randomly according to

$$d\mathcal{P}[p^n(t + \Delta t) = p] = S(p, p^{n0}(t + \Delta t)) dp$$

So  $S(p, q)$  is the probability density that  $q \rightarrow p$  in the time interval  $\Delta t$ . This is the complicated part of the Monte Carlo code. However, it does not really concern you since we are only going to modify Step 1. So it would be ideal if you could use Step 2 as a 'black box', if this is possible.

## 2 Modifying MC using effective potentials

O.k. this was classical transport, where we have essentially dealt with the electron as a pin ball flying around in a pinball machine and bumping into obstacles. (The only exception being the relation between velocity and  $p$ ; that's why its called semi-classical transport.) Now we are trying to include quantum effects. For the background on the quantum transport equations you best read the reference paper by Ringhofer, Gardner, Vasileska (I think you have it; if not, it is on my web-page). The point of the whole exercise, as far as implementation goes, is that the potential  $V$  in (3) is replaced by an 'effective quantum potential'. Other than the classical potential  $V$ , this potential  $V^Q$  is actually a function of position and momentum, and (3) is replaced by

$$x^n(t + \Delta t) = x^n(t) + \Delta t \nabla \varepsilon(p^n(t)), \quad p^{n0}(t + \Delta t) = p^n(t) - \Delta t e \nabla_x V^Q(x^n, p^n, t) \quad (4)$$

So, the only two things you have to figure out is where in Shaikh's code you replace (3) by (4), and how to compute the quantum potential  $V^Q$  from the original potential  $V$ , which in Shaikh's code is computed from the Poisson equation. The quantum potential  $V^Q$  is given as convolution of the original potential  $V$  with a kernel. I find it useful to use the notation of pseudo - differential operators. In this notation  $V^Q$  is given as

$$V^Q(x, p, t) = \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] \frac{2m \sin\left[\frac{\beta \hbar p \cdot \nabla_x}{2m}\right]}{\beta \hbar p \cdot \nabla_x} V(x, t) \quad (5)$$

## INSERT: A bit on pseudo - differential operators (PDO's)

We are using PDO's here essentially as a compact notation to write integral convolution operators. (Mathematically, there is actually much more to it. You are going to use them in the math. part of your dissertation. So you might as well get used to them.) The general principle is that you have a symbol (i.e. a function of two variables)  $A(x, z)$ . You apply the PDO  $A(x, \nabla_x)$  to a function  $V(x)$  by

- 1) replacing  $\nabla_x$  by  $i\xi$ . Here  $\xi$  is the frequency variable corresponding to  $x$  in the Fourier transform,
- 2) You multiply  $A(x, i\xi)$  with the Fourier transform  $\hat{V}(\xi)$ .
- 3) You back Fourier transform.

So this means:

$$A(x, \nabla_x)V(x) = \int A(x, i\xi)\hat{V}(\xi)e^{i\xi \cdot x} d\xi, \quad \hat{V}(\xi) = (2\pi)^{-d} \int V(y)e^{-iy \cdot \xi} dy \quad (6)$$

$d$  here is the dimension of  $x$ , i.e.  $d = 1$  or  $d = 2$  in Shaikh's code.

Obviously, if  $A(x, \nabla_x)$  is a polynomial in  $\nabla_x$ , then this reduces to the usual definition of a linear differential operator. As an exercise, to get used with the notation, prove the following statement for yourself:

*$A(x, \nabla_x)$  maps real functions into real functions if and only if  $A(x, \nabla_x) = A(x, -\nabla_x)^*$  holds. (i.e. the real part of  $A$  is an even function and the imaginary part of  $A$  is an odd function of  $\nabla_x$ ).*

(Since the symbol in (5) is real and even, this works.) With this notation (5) becomes

$$V^Q(x, p, t) = \int \exp\left[-\beta \frac{\hbar^2 |\xi|^2}{8m}\right] \frac{2m \sinh\left[\frac{\beta \hbar p \cdot \xi}{2m}\right]}{\beta \hbar p \cdot \xi} \hat{V}(\xi, t) e^{i\xi \cdot x} d\xi, \quad \hat{V}(\xi, t) = (2\pi)^{-d} \int V(y, t) e^{-iy \cdot \xi} dy \quad (7)$$

(remember from calculus that  $\sin(iz) = i \sinh(z)$  holds!)

**END OF INSERT**

## 3 How to evaluate the effective potentials

So, we have to compute  $V^Q$  from  $V$  according to (5) and put it into Shaikh's code in the formula (2). Actually, there are two potentials we are dealing with:

- One is the barrier potential  $V_B(x)$ , which models the  $Si - SiO_2$  interface. This potential

is one- dimensional (i.e. depends only on the  $x$ - component orthogonal to the interface.) and independent of time.

- The second is the Hartree potential  $V_H(x, t)$ , computed from Poisson's equation, which is two - dimensional and time dependent.

$$V^Q(x, p, t) = V_B^Q(x, p) + V_H^Q(x, p, t),$$

$$V_B^Q(x, p) = \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] \frac{2m \sin\left[\frac{\beta \hbar p \cdot \nabla_x}{2m}\right]}{\beta \hbar p \cdot \nabla_x} V_B(x), \quad V_H^Q(x, p, t) = \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] \frac{2m \sin\left[\frac{\beta \hbar p \cdot \nabla_x}{2m}\right]}{\beta \hbar p \cdot \nabla_x} V_H(x, t) \quad (8)$$

Although this split seems artificial, the two have to be treated differently for the following practical computational reason: Since  $V^Q(x, p, t)$  has to be evaluated for all electron positions and momenta  $x^n, p^n$ ,  $n = 1, \dots, N$ , in (2), and  $N$ , the number of electrons is large, we cannot compute the convolution integral in (5)  $N$  times at each time step. On the other hand, the barrier potential  $V_B^Q$  does not change in time and is only one - dimensional. So we can do this once, tabulate it and use the table values. For the Hartree part this is not practically feasible, since it would have to be done at each time step. So, here we have to use an approximation to (5).

### The barrier potential:

The barrier potential is just a step function. So  $e \nabla_x V_B(x) = B(1, 0, 0)^T \delta(x_1)$  holds. Here  $x_1$  is the direction orthogonal to the interface and  $B$  is the barrier height (something like  $4eV$ ). We actually need only the gradients of the potential. So we really compute

$$\nabla_x V_B^Q(x, p) = \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] \frac{2m \sin\left[\frac{\beta \hbar p \cdot \nabla_x}{2m}\right]}{\beta \hbar p \cdot \nabla_x} \nabla_x V_B(x)$$

This gives, according to (6)

$$e \widehat{\nabla_x V_B}(\xi) = \frac{B}{2\pi} \delta(\xi_2) \delta(\xi_3) (1, 0, 0)^T,$$

$$e \nabla_x V_B^Q(x, p) = \frac{B}{2\pi} (1, 0, 0)^T \int \exp\left[-\beta \frac{\hbar^2 |\xi_1|^2}{8m}\right] \frac{2m \sinh\left[\frac{\beta \hbar p_1 \cdot \xi_1}{2m}\right]}{\beta \hbar p_1 \cdot \xi_1} e^{i \xi_1 \cdot x_1} d\xi_1 \quad (9)$$

Note that  $V_B^Q$  is only a function of  $x_1, p_1$ , i.e. it remains strictly one dimensional. This, and the fact that we only do it once, is the reason we can actually tabulate the formula (9) on a mesh. **Now this is already done and Shaikh has the code for it!**

### The Hartree potential:

So here is where the actual work starts for you. So Shaikh's code produces from Poisson's equation a classical Hartree potential  $V_H(x_1, x_2, t)$  given on a rectangular mesh, and we have to evaluate  $V_H^Q(x_1, x_2, p_1, p_2, t)$  according to (8) for all particle positions and momenta  $x^n, p^n$ ,  $n = 1, \dots, N$ . This is of course impossible to do in finite time.

My first suggestion is the following: The quantum potential is evaluated by multiplying the Fourier transform of the potential by a function of  $\hbar\xi$ . The smoother  $V(x)$ , the faster  $\hat{V}(\xi)$  will decay in  $\xi$ . Thus, for smooth  $V$  it is reasonable to approximate the whole thing for small  $\xi$ . Remember,  $\hbar$  is small which helps. This should work for the Hartree potential, since it is a reasonably smooth function. The barrier potential is another matter. So expanding the  $\frac{\sin(z)}{z}$  term in (8) gives

$$V_H^Q(x, p, t) \approx \left[1 - \frac{\beta^2 \hbar^2 (p \cdot \nabla_x)^2}{24m^2}\right] \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] V_H(x, t),$$

Which would lead to the following algorithm: Given  $V_H(x, t)$  on a mesh

Step 1:

Compute  $V_H^0(x, t)$  on the same mesh according to

$$V_H^0(x, t) = \exp\left[\beta \frac{\hbar^2 |\nabla_x|^2}{8m}\right] V_H(x, t),$$

Now this is easy, since  $V_H^0$  does not depend on the momentum  $p$ . It can be done either by using the Fourier transform definition (6) or by direct convolution with a Gaussian. Using (6), we obtain

$$V_H^0(x, t) = (2\pi)^{-2} \int \exp\left[-\beta \frac{\hbar^2 |\xi|^2}{8m}\right] V_H(y, t) \exp[i\xi \cdot (x - y)] dy d\xi = \int \Gamma(x - y) V_H(y, t) dy, \quad (10)$$

$$\Gamma(z) = (2\pi)^{-2} \int \exp\left[-\beta \frac{\hbar^2 |\xi|^2}{8m}\right] \exp[i\xi \cdot z] d\xi = (2\pi)^{-1} \frac{4m}{\beta \hbar^2} \exp\left[-\frac{2m|z|^2}{\beta \hbar^2}\right]$$

( $x, y, \xi$  are all 2-dimensional and we use the fact that the function  $e^{-z^2/2}$  is its own Fourier transform.) So you can compute  $V_H^0$  using discrete Fourier transforms or evaluating the convolution (10) directly.

Step 2:

Once you have  $V_H^0(x, t)$  on the mesh, evaluate the components of  $\nabla_x V_H^Q$  according to

$$\partial_{x_r} V_H^Q(x^n, p^n, t) = \partial_{x_r} V_H^0(x^n, t) - \frac{\beta^2 \hbar^2}{24m^2} \sum_{j,k=1}^2 p_j^n p_k^n \partial_{x_j} \partial_{x_k} \partial_{x_r} V_H^0(x^n, t), \quad n = 1, \dots, N \quad (11)$$

for all particles. This is done simply by numerical differentiation of the sufficiently smooth grid function  $V_H^0$  and interpolation.

## 4 Some subtle questions:

1. What is  $\beta$ ?

This is a subtle question.  $\beta$  is in dimensions a reciprocal energy. In the derivation of the

quantum potential  $\beta$  is actually a constant, namely room temperature  $\frac{1}{k_b T} \approx 40(eV)^{-1}$ . Now to use this value in the barrier potential (9) turned out to be numerically absolutely impossible. So, currently in Shaikh's code, we use the electron temperature for  $\beta = \frac{2m}{|p|^2}$  which makes  $V_B^Q$  actually a function of three variables,  $V_B^Q(x_1, p_1, \beta)$  which has to be tabulated (once) for all relevant values. Now for the Hartree potential formula (11) you can probably use the constant room temperature value  $40(eV)^{-1}$ .

2. Why not use the same approach in (11) for both  $V_B$  and  $V_H$ ?

Well, even the barrier is sufficiently smooth once it is convoluted with the Gaussian  $\Gamma$  in (10). So, you might experiment with that. The truth is, I did not think of this simple way before. The smoothing in the Hartree potential will not make much of a difference. The smoothing in the barrier is the important part. So the gradient approximation is more of a question. But you can try this easily once you have the code for the Hartree potential.