Journal of Computational and Theoretical Nanoscience
Vol. 8, 1–6, 2011

Numerical Solution and Statistically Analysis for Estimation of the Heat Flux in Thermal Scanning Process Using Conjugate Gradient Method

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Heat flux in process of thermal scanning is investigated using the inverse algorithm by conjugate gradient method. The numerical results is shown for four values of standard deviation $\sigma = 0.1$, 0.5, 1 and 2. The analysis of error is presented for various σ and number of iteration. It is found that as $\sigma > 0.1$ there are an optimum range for number of iteration that the values of error are at minimum.

Keywords: Nano Scale Scanning and Wiring, Thermal Microscopy, Heat Flux Estimation, Conjugate Gradient Method.

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1. INTRODUCTION

The invention of scanned probe microscopes in the 1980s revolutionized atomic-scale imaging and spectroscopy. In particular, scanning tunneling and atomic force microscopes (STM and AFM) have found widespread applications in physics, chemistry, material science, and biology. The possibility of atomic-scale manipulation, lithography, and nano-machining using such probes was considered from the beginning and has matured considerably over the past decade. In normal operation, an atomic force microscope (AFM) allows to obtain a topographic image of a surface with nanometer spatial resolution. If the tip of the AFM is thermally active, in addition it will readily produce a thermal image, which is the basis of scanning thermal microscopy (SThM).[1–5] Scanning thermal microscopy (SThM) where the tip is used to heat the sample and sense heat flow out of the probe, surface topography and surface modification nanoscale thermal imaging, to biomolecular sensing, atomic-level detection and nanolithography. Also, SThMs can be used for writing by melting the substrate thermally data storage.[6] Joule (e.g., Ref. [7]) or Peltier heating (e.g., Ref. [8]) have presented various methods for heating the extremity of the tip. Fonseca et al.[9] has been used an atomic force microscope (AFM) with an integrated thermal sensor to obtain the local spatial distribution of temperatures in a micro-machined thermopile with submicron resolution. Although accurate absolute local temperature measurements are difficult to obtain from this technique, it offers unique possibilities when qualitatively comparing areas with a temperature contrast. As before mentioned, one of important applications of thermal microscopes is nanoscale wiring by both AFM (Atomic Force Microscope) tip and laser beam. Being able to make a relatively small deflection, a micro thermal actuator can be used to control the near field optics of the beam minutely and accurately. In the current study, an algorithm based on conjugate gradient method (CGM) is applied to estimate the unknown heat flux entered the sample.

2. ANALYSIS

In many dynamic heat transfer situations, the surface heat flux and temperature histories of a solid must be determined from transient temperature measurements at one or more interior locations; this is an inverse problem.[10–11] Figure 1 shows the geometry of the problem. The thermal conductivity k, density ρ, and specific heat c are postulated to be known and constant. The initial temperature distribution T_0 is also taken as known. The location $x = 0$ of the sensor is inactive surface and adiabatic. The algorithm based on conjugate gradient method (CGM) is applied to estimate the unknown heat flux $q''(t)$, entering the active surface at $x = L$ and there is no any information about the history of unknown heat flux.

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 1546-1955/2011/8/001/006 doi:10.1166/jctn.2011.1741

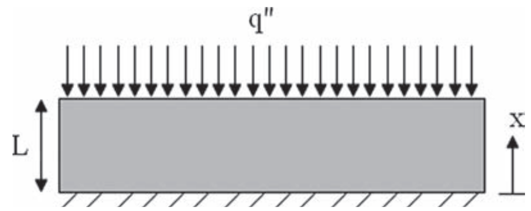

Fig. 1. A schematic for the problem.

2.1. Direct Problem

To estimate the surface heat flux history it is necessary to have a mathematical model of the heat transfer process. A possible mathematical model for the temperature $T(x, t)$ in the plate is:

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = \rho c\frac{\partial T}{\partial t} \tag{1}$$

With initial condition:

$$T(x, t) = T_0 \tag{2}$$

And boundary conditions:

$$\left.\frac{\partial T(x, t)}{\partial x}\right|_{x=0} = 0 \tag{3}$$

$$-k\left.\frac{\partial T(x, t)}{\partial x}\right|_{x=L} = q''(t) \tag{4}$$

2.2. Inverse Problem

The solution of the direct problem with the unknown heat flux $q''(t)$ can be treated as a problem of optimum control, which has the control function $q''(t)$ and is intended to minimize the functional $S(q''(t))$ defined as

$$S(q''(t)) = \sum_i [Y_i - T_i]^2 \tag{5}$$

where T_i is the exact temperature at $x = 0$

$$S(\vec{\beta}+\lambda\vec{S}) = \sum_i [Y_i - T_i(\vec{\beta}+\lambda\vec{S})]^2 \tag{6}$$

where $\vec{\beta}$ is base point of minimization process, λ is step size and $\vec{S}$ is search direction that is $-\vec{\nabla}S$ for minimization. To minimize the function S:

$$\frac{\partial S}{\partial \lambda} = 0 \tag{7}$$

Then optimum step size λ^* is obtained from follow:

$$\lambda^* = \frac{\sum_i [Y_i - T_i(\vec{\beta})]\Delta T_i}{\sum_i \Delta T_i^2} \tag{8}$$

2.3. Sensitivity Equation

In order to determine ΔT, change $\vec{\beta}$ to $\vec{\beta}+\Delta\vec{\beta}$ that will cause a change: $T \to T+\Delta T$ in the Eq. (1) by setting this changes in the model Eqs. (1–4) sensitivity equation can be obtained as follow:

$$k\left(\frac{\partial^2 \Delta T}{\partial x^2}\right) = \rho c\frac{\partial(\Delta T)}{\partial t} \tag{9}$$

with initial condition:

$$\Delta T\,|_{t=0} = 0 \tag{10}$$

And boundary conditions:

$$\left.\frac{\partial(\Delta T)}{\partial x}\right|_{x=0} = 0 \tag{11}$$

$$\left.\frac{\partial(\Delta T)}{\partial x}\right|_{x=L} = \Delta q''(t) \tag{12}$$

2.4. Adjoin Differential Equation

Lagrange method is used for constrained optimization. By definition Lagrange's function as follow:

$$L(T, \vec{q}) = \int_{t=0}^{t_f}\int_{x=0}^{L} [Y-T]^2\delta(x-x_s)\,dx\,dt + \int_{t=0}^{t_f}\int_{x=0}^{L} \lambda(x, t)\left[\frac{\partial^2 T}{\partial x^2} - \frac{\partial T}{\partial t}\right]dx\,dt \tag{13}$$

where $\delta(x-x_s)$ is Dirac function and x_s is sensor location. Taking variation of L and setting equal zero the Adjoin differential equation is obtained:

$$\frac{\partial^2\lambda}{\partial x^2} + \frac{\partial\lambda}{\partial t} + 2[T-Y]\delta(x-x_s) \tag{14}$$

with initial condition:

$$\lambda\,|_{t=t_f} = 0 \tag{15}$$

And boundary conditions:

$$\left.\frac{\partial\lambda}{\partial x}\right|_{x=0} = 0 \tag{16}$$

$$\left.\frac{\partial\lambda}{\partial x}\right|_{x=L} = 0 \tag{17}$$

Using Adjoin differential equation and variation of L:

$$\Delta S = \int_{t=0}^{t_f} \lambda(0, t)\delta q\; dt \tag{18}$$

From above equation it can be found $\vec{\nabla}S = \lambda(0, t)$.

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3. NUMERICAL RESULT AND DISCUSSION

Results are obtained by using mentioned numerical procedure and for copper with heat capacity $\rho c = 3.546 \times 10^6$ j/m^3 °K, thermal conductivity $k = 373$ W/m °K for $T = 400$ °K. The length L is choosing 100 μm. The measurement of the temperature in surface position is necessary for estimating the melt depth. If a computer simulation is used, the temperatures involve random measurement errors and random noise is added to the error-free simulated data to generate the measured temperatures; that is: $(Y(0,t) = T(0,t) + \textit{Noises normal distribution})$ where $T(0,t)$ is the surface temperature of the direct problem.

$$P(\chi) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[\frac{-1}{2}\left(\frac{\chi}{\sigma}\right)^2\right] \tag{19}$$

where $P(\chi)$ is probability density function for normal distribution. In Eq. (19) it is assumed than all data not having

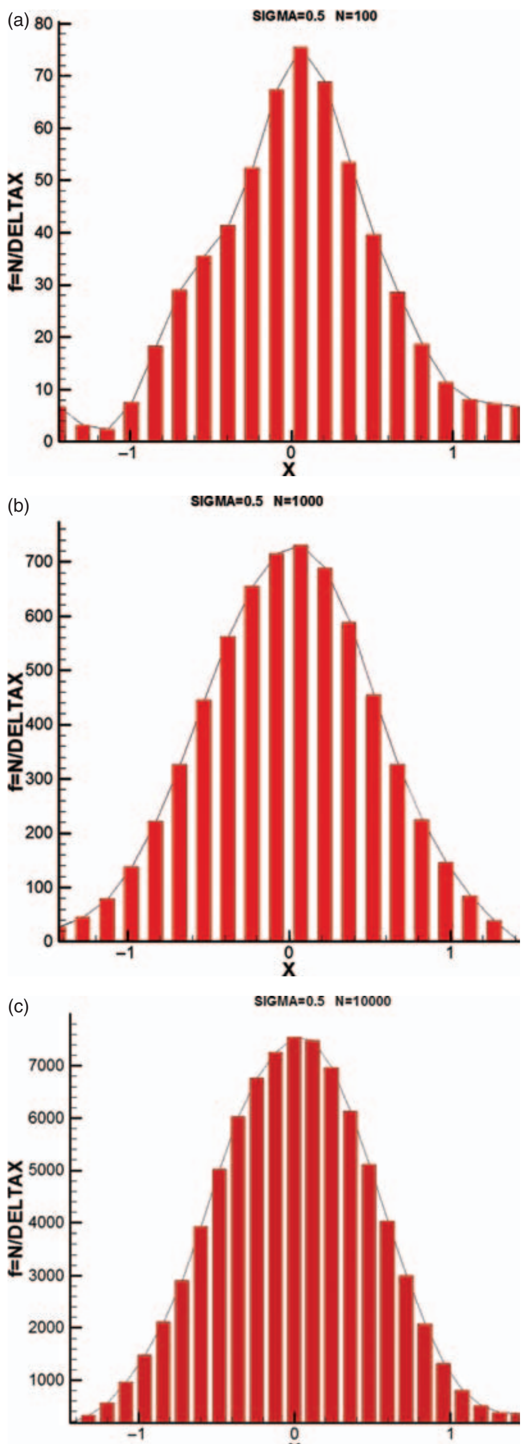

Fig. 2. Gaussian distribution of noise of temperature verses number of data: (a) $N = 100$, (b) $N = 1000$ and (c) $N = 10,000$.

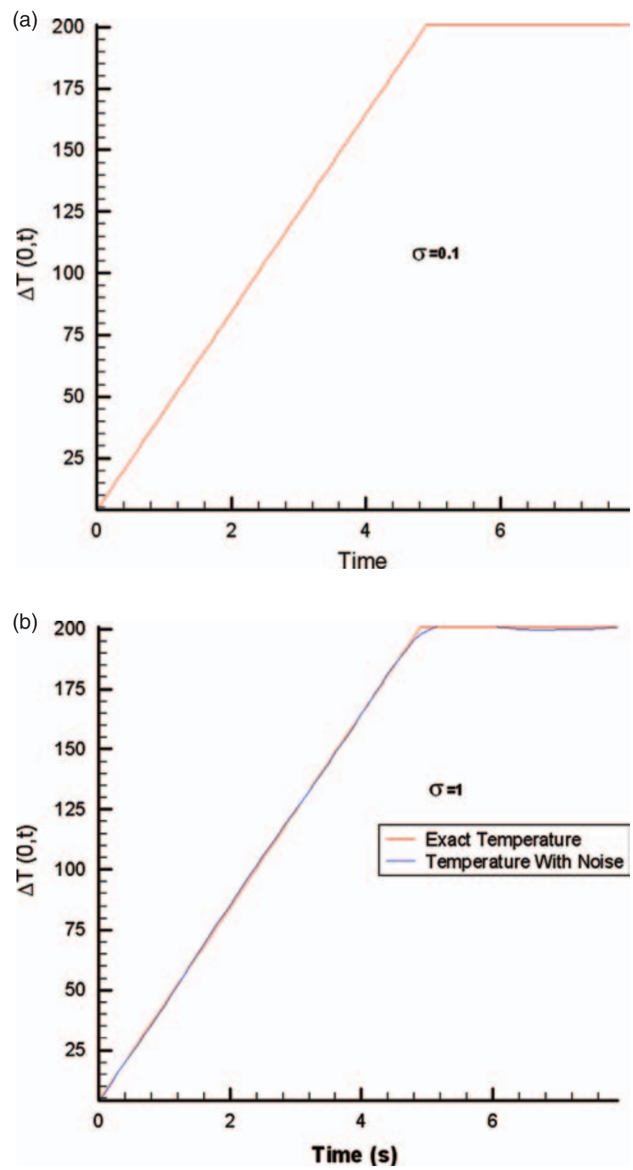

Fig. 3. Exact temperature and temperature with noise verses time: (a) $\sigma = 0.1$, $\sigma = 1$.

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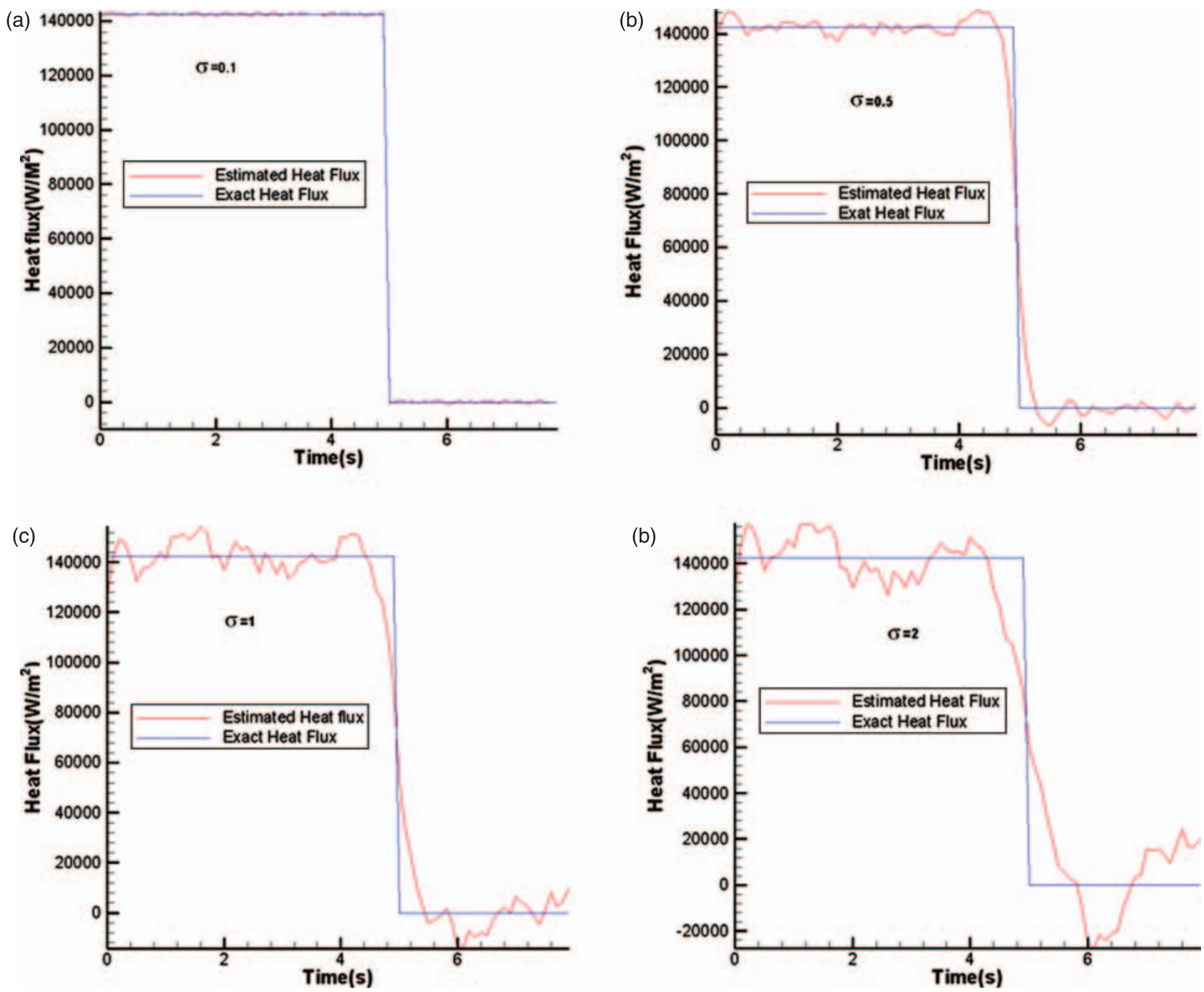

Fig. 4. Estimated and exact heat flux verses time: (a) $\sigma = 0.1$, (b) $\sigma = 0.5$, (c) $\sigma = 1$, (d) $\sigma = 2$.

mean value. Product errors using Mounte Carlo method are obtained from follow integration:

$$R(\chi) = \int_{-\infty}^{\chi} P(\chi')d\chi' \tag{20}$$

Form this method a random number $0 < R < 1$ is substituted instead of $R(\chi)$, and using Eq. (20) χ will be obtained. With finding many number of χ, it is found that all of χ have normal distribution. Figure 2 shows Gaussian (Normal) distribution of noise of temperature verses number of data (N). It is found as number of data increases distribution of data is smoother.

Figure 3 shows the temperature difference from initial temperature for exact temperature and temperature with noise verses time, for $\sigma = 0.1$. Because of noises are low the exact temperature and temperature with noise are same.

In order to estimate heat flux from the Inverse Heat Conduction algorithm a known heat flux is exerted to active surface. Then using direct solution, exact temperatures verses Time are obtained and random noise is added to the error-free simulated data to generate the measured temperatures. Variations of measured temperatures are inputs of inverse algorithm.

Variations of estimated and exact heat flux verses time is presented in Figure 4. It can be seen as $\sigma = 0.1$ estimated and exact heat flux approximately have same value and the result are excellent and as σ increase in order to values of noise increases the results become few different from exact heat flux.

4. ERROR ANALYSIS

To investigate of error in the problem follow concepts are defined:

$$\text{ERMS}^2 = \frac{1}{n}\sum_{M=1}^{N}(\hat{q}_M - q_M)^2 \tag{21}$$

where $\hat{q}_M$ is estimated heat flux and q_M is exact Heat flux. And:

$$\text{BAIAS}^2 = \frac{1}{n}\sum_{M=1}^{N}(\hat{q}_{M,W} - q_M)^2 \tag{22}$$

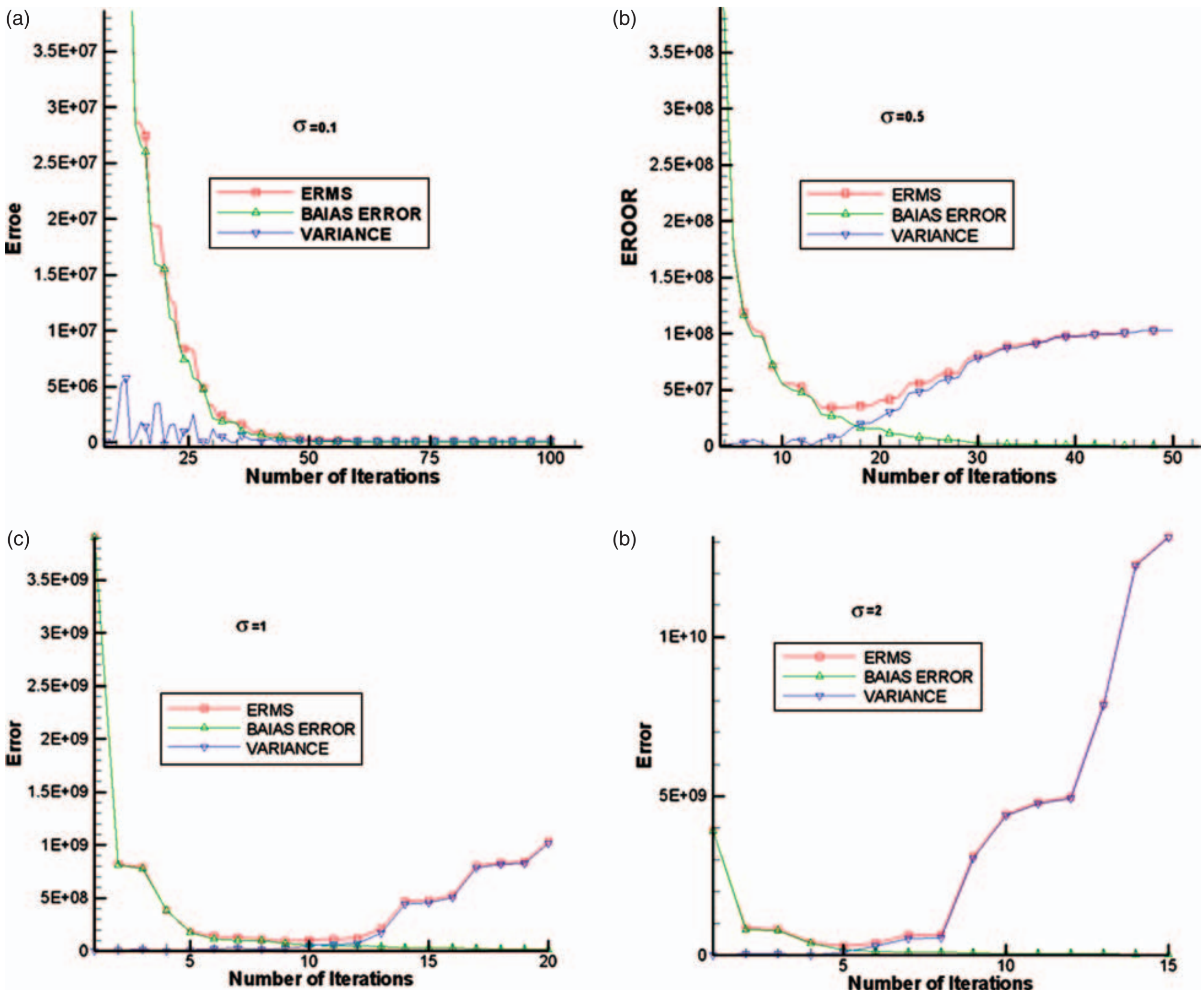

Fig. 5. ERMS, BAIS and VARIANCE verses Time: (a) $\sigma = 0.1$, (b) $\sigma = 0.5$, (c) $\sigma = 1$, (d) $\sigma = 2$.

where $\hat{q}_{M,W}$ is estimated heat flux without noise, and

$$\text{VARIANCE}^2 = \text{ERMS}^2 - \text{BAIAS}^2 \tag{23}$$

These concepts are plotted in Figure 5, and for more easy investigation those powers are not showed in the figure but the values are in square. From Figure 5 it can bee found as the values of σ increases errors increased. The important note is that for $\sigma = 0.1$ (low standard deviation) when number of equation increases, errors decreased and the values of error become zero, for number of equation greater than 50. But when standard deviation increase for example greater than 0.5, there are a range optimum values for number of equation that the values of errors are at minimum and if values of errors have a crossover point this point is optimist number of iteration.

5. CONCLUSION

In current study a numerical inverse algorithm (CGM method) is used to estimate an unknown Heat flux in process of thermal scanning of an AFM or SThM or other applications. The results is shown for four values of standard deviation $\sigma = 0.1$, 0.5, 1 and 2. It is found that as $\sigma > 0.1$ there are an optimum range for number of iteration that the values of error are at minimum.

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Received: 2 February 2009. Accepted: 23 March 2009.

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