2D Heat Equation Modeled by Crank-Nicolson Method

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1 The Heat Equation

$$\frac{\partial U}{\partial t} - \alpha \frac{\partial^2 U}{\partial x^2} = 0 \qquad \frac{\partial U}{\partial t} - \alpha \, \nabla^2 \mathbf{x} = 0$$

The system I chose to study was that of a hot object in a cold medium, and document the time progression of various cases. This system is fairly straight forward to relate to as it a situation we frequently encounter in daily life. Heat transfer follows a few classical rules:

-Heat flows from hot to cold (Hight T to low T)

-Heat flows at rate proportional to the temperature difference. This rate is α

-A change in heat results in a change in T

$\Delta T = mC_vQ$

-Total heat energy must be conserved.

Such systems in general are equilibrium seeking, non-oscillatory systems which approach the equilibrium state (constant T) asymptotically as time progresses.

In my system we consider a grid of 100x100 particles with $m = C_v = 1$ and constant α across the whole grid. While this system is rather simplistic, it still allows us to model and solve many complex and interesting distributions of heat features.

In addition, this model can easily be extended to other non-heat related systems. Namely:

-Diffusion of a particle density function P

$$\partial_t P = D\,\nabla^2 P$$

-Schrdinger equation of a free particle

$$\partial_t \psi = \frac{i\hbar}{2m}\nabla^2 \psi$$

2 The Crank-Nicolson Method

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}[F_i^{n+1}(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}) + F_i^n(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2})]$$

Where: $\frac{\partial u}{\partial t} = F(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2})$

The Crank-Nicolson Method (CNM) can be thought of as a combination of the forward and backward Euler methods, but it should not be mistaken as a simple average of the two as the method is implicitly dependent on its solution. (Much like backwards Euler, but differing from forward Euler).

This method is a good choice for solving the heat equation as it is unconditionally stable for both 1D and 2D applications. This trait makes it ideal for any system involving a conservation law.

2.1 1D Crank-Nicolson

In one dimension, the CNM for the heat equation comes to:
(n is the time step, i is the position):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{a}{2(\Delta x)^2}[(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + (u_{i+1}^n - 2u_i^n + u_{i-1}^n)]$$

which allowing $r = \frac{a\Delta t}{2(\Delta x)^2}$ simplifies to:

$$-ru_{i+1}^{n+1} + (1 + 2ru_i^{n+1}) - ru_{i-1}^{n+1} = ru_{i+1}^n + (1 - 2ru_i^n) + ru_{i-1}^n$$

which can be solved for u_i^{n+1} rather simply from the equation:

$$\mathbf{A} * \bar{\mathbf{u}}^{\mathbf{n+1}} = \mathbf{B} * \bar{\mathbf{u}}^{\mathbf{n}}$$

where A and B are tridiagonal matrices and $\bar{\mathbf{u}}^{\mathbf{n}}$ is the vector representation of the 1D grid at time n.

2.2 2D Crank-Nicolson

In two dimensions, the CNM for the heat equation comes to:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{a}{2(\Delta x)^2}[(u_{i+1,j}^{n+1}+u_{i-1,j}^{n+1}+u_{i,j+1}^{n+1}+u_{i,j-1}^{n+1}-4u_i^{n+1})+(u_{i+1,j}^{n}+u_{i-1,j}^{n}+u_{i,j+1}^{n}+u_{i,j-1}^{n}-4u_i^{n})]$$

assuming $\Delta x = \Delta y$ and letting $\mu = \frac{a\Delta t}{(\Delta x)^2}$ gives us:

$$(1+2\mu)u_{i,j}^{n+1}-\frac{\mu}{2}(u_{i+1,j}^{n+1}+u_{i-1,j}^{n+1}+u_{i,j+1}^{n+1}+u_{i,j-1}^{n+1}) = (1-2\mu)u_{i,j}^{n}+\frac{\mu}{2}(u_{i+1,j}^{n}+u_{i-1,j}^{n}+u_{i,j+1}^{n}+u_{i,j-1}^{n})$$

or if we allow the use of the operators δ_x^2 and δ_y^2 where:

$$\delta_x^2 f_{i,j} = f_{i+1,j} - 2f_{i,j} + f_{i-1,j} \qquad \delta_y^2 f = f_{i,j+1} - 2f_{i,j} + f_{i,j-1}$$

the equation can be written as

$$(1 - \frac{\mu}{2}\delta_x^2 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2 + \frac{\mu}{2}\delta_y^2)u_{i,j}^{n}$$

which is very nice and pretty, but not too much fun solve. So we go in search of a different equation to solve. Let us consider:

$$(1 - \frac{\mu}{2}\delta_x^2)(1 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2)(1 + \frac{\mu}{2}\delta_y^2)u_{i,j}^{n}$$

which can be shown to be a fair approximation of the original equation if you consider quadratic terms negligible.

$$(1 - \frac{\mu}{2}\delta_x^2 - \frac{\mu}{2}\delta_y^2 + \cancelto{0}{\frac{\mu}{2}\delta_y^2\frac{\mu}{2}\delta_x^2})u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2 + \frac{\mu}{2}\delta_y^2 + \cancelto{0}{\frac{\mu}{2}\delta_y^2\frac{\mu}{2}\delta_x^2})u_{i,j}^{n}$$

The advantage of this new form is that it allow us to solve in two steps with the help of an intermediate value u^*

$$(1 - \frac{\mu}{2}\delta_x^2)u_{i,j}^* = (1 + \frac{\mu}{2}\delta_y^2)u_{i,j}^n$$

$$(1 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2)u_{i,j}^*$$

which is confirmed to be a valid method by multiplying the upper by $(1 + \frac{\mu}{2}\delta_x^2)$ and the lower by $(1 - \frac{\mu}{2}\delta_x^2)$ which yields:

$$(1 - \frac{\mu}{2}\delta_x^2)(1 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2)(1 - \frac{\mu}{2}\delta_x^2)u_{i,j}^* = (1 + \frac{\mu}{2}\delta_x^2)(1 + \frac{\mu}{2}\delta_y^2)u_{i,j}^n$$

$$(1 - \frac{\mu}{2}\delta_x^2)(1 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_x^2)(1 + \frac{\mu}{2}\delta_y^2)u_{i,j}^n$$

which is exactly what we were going for. This 2 step process allows us to handle 1 dimension at a time which allows the use of matrix notation just like before, almost. By naively solving the 1D case twice, we would be tempted to solve for

$$(1 - \frac{\mu}{2}\delta_x^2)u_{i,j}^* = (1 + \frac{\mu}{2}\delta_x^2)u_{i,j}^n$$

$$(1 - \frac{\mu}{2}\delta_y^2)u_{i,j}^{n+1} = (1 + \frac{\mu}{2}\delta_y^2)u_{i,j}^*$$

which looks close, but is not correct. The issue lies in that previously, we were always taking derivatives in the same dimension we were evaluating, i.e. taking x derivatives along the x axis of a vector or matrix. But now we have to compare the δ_x^2 and δ_y^2 operators. Naturally we chose to evaluate a whole row/column of the grid at once, and so the operator in the same direction is easy (matrix-vector multiplication like in 1D) but the other operator gives us some trouble. The issue with the off-axis operator is that unlike the on-axis operator the j+1 and j-1 terms are not on the row/column you are currently evaluating, and so could not simply be solved using traditional vector/matrix multiplication since as those j+1 and j-1 values would not be in the vector.

A solution becomes clear when we take a step back, and realize we don't need to try and find some matrix-like solution, rather all we needed is the vector result of the operator, and so we can simply apply the off-axis operator via the roll function. Once we have the off-axis operator figured, the rest of the program falls into place and we are ready to test.

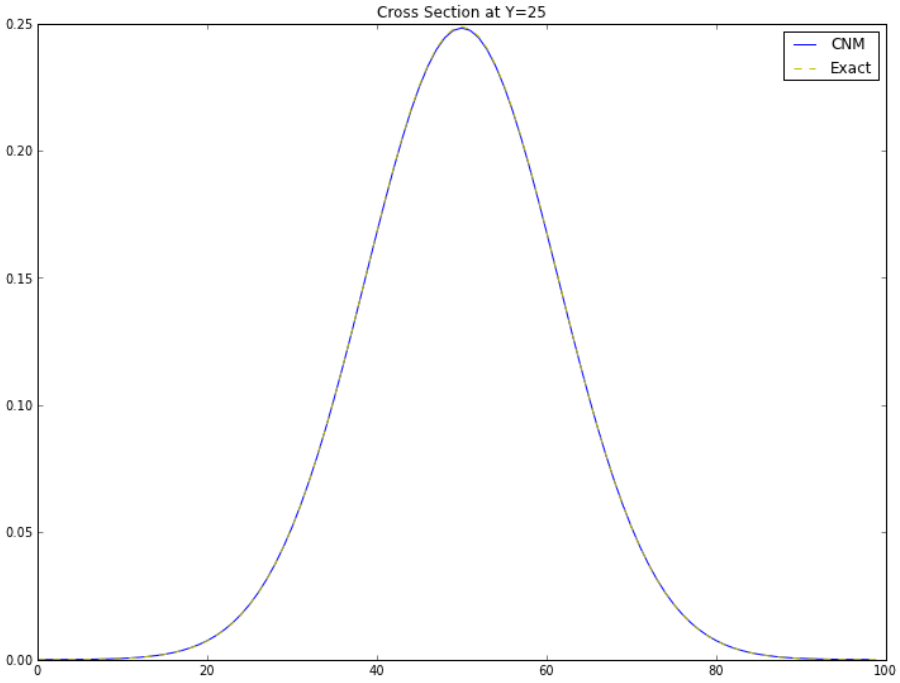
3 Testing

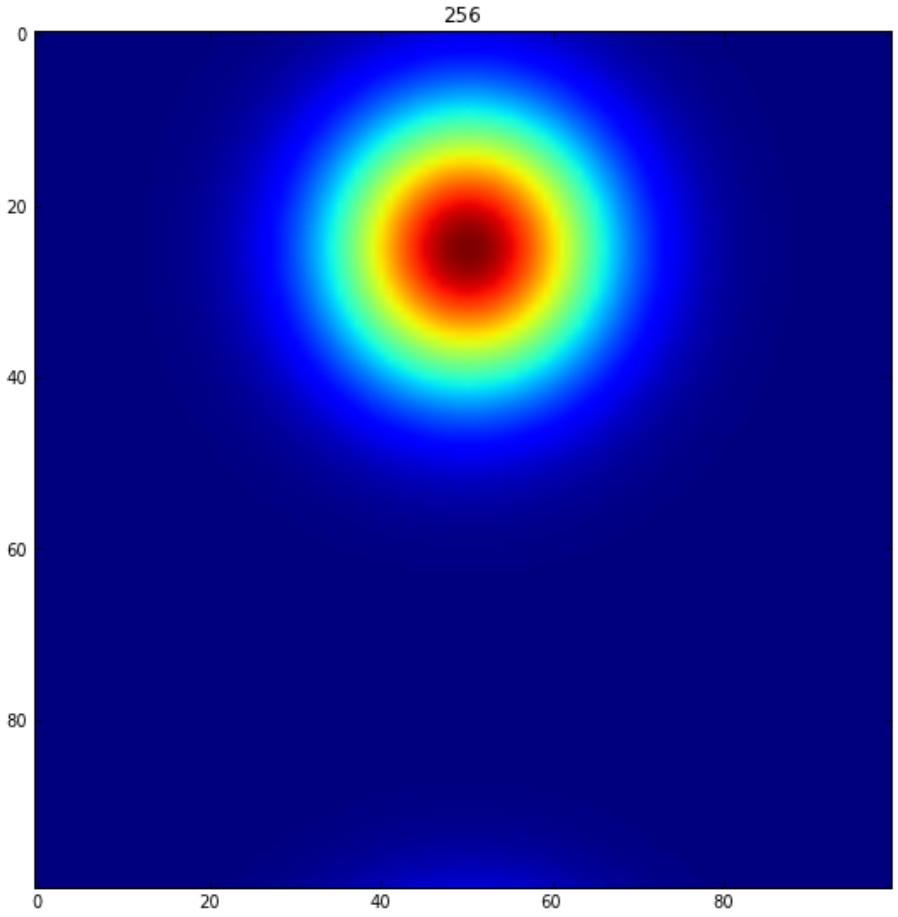
3.1 Numeric Accuracy

To test our system we can compare it to the analytical solution of a delta function:

$$u(r,t) = T_o \frac{\alpha e^{-r^2}}{4\pi t}$$

where r is the distance from the origin centered at the delta function. In our model a delta function is approximated as one hot square in a bath of T=0. The weight of the delta function (T_o) is equal to $T_g(\Delta x)^2$ where T_g is the temperature of the hot grid point. This is to ensure that the integral over all the grid (Total Energy) is the same for both cases. The results after 256 steps with $\Delta t = .25$ yielded an error of $1.44 * 106{-}4$ of and a variance of $2.293{*}10^{-8}$. It can be seen from the heat map that the results are rotationally symmetric about the delta function, as predicted.

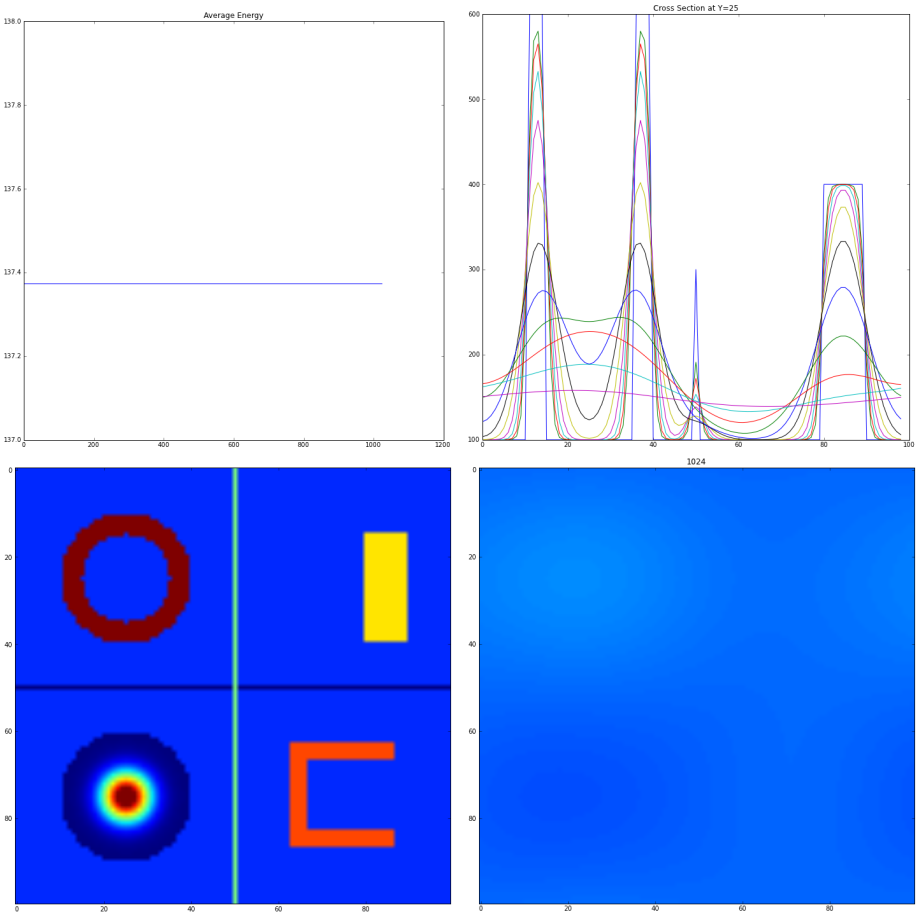




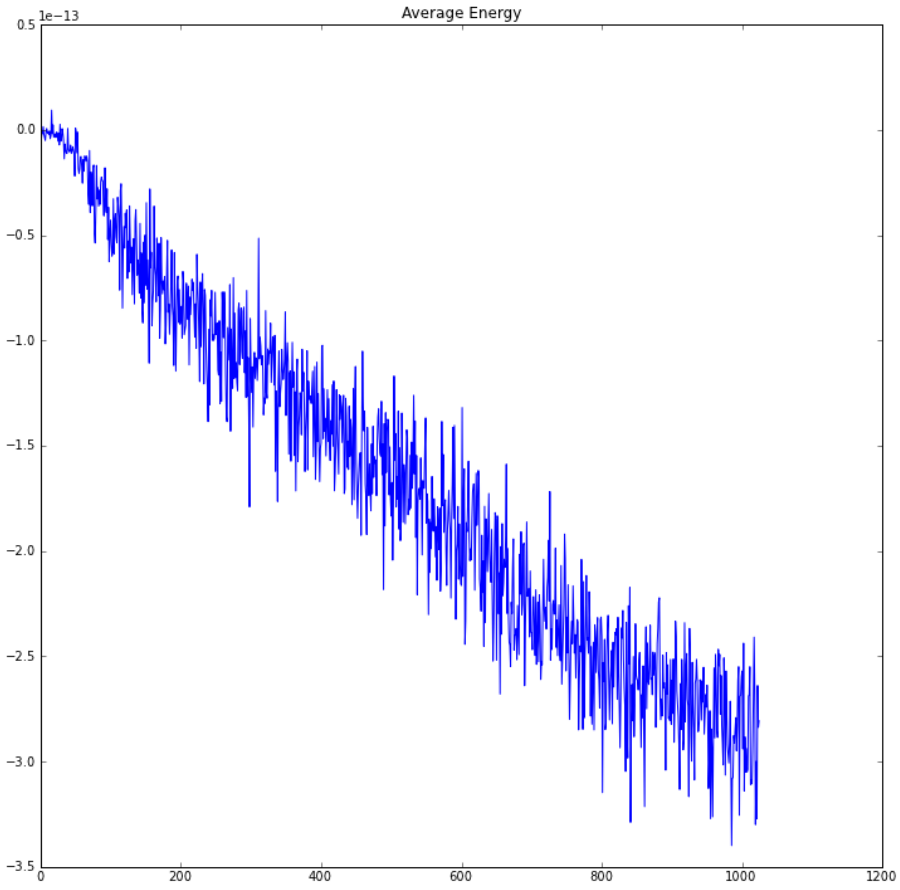
After testing for a few differing values of Δx and α we become satisfied with the accuracy of the simulation given $\Delta t = .25$, which will be the default unless otherwise noted.

3.2 Energy Conservation

We then can go on to test the energy conservation of our system. For a test run of 1024 steps with a complex initial heat map we find the average energy of the system to stay constant!

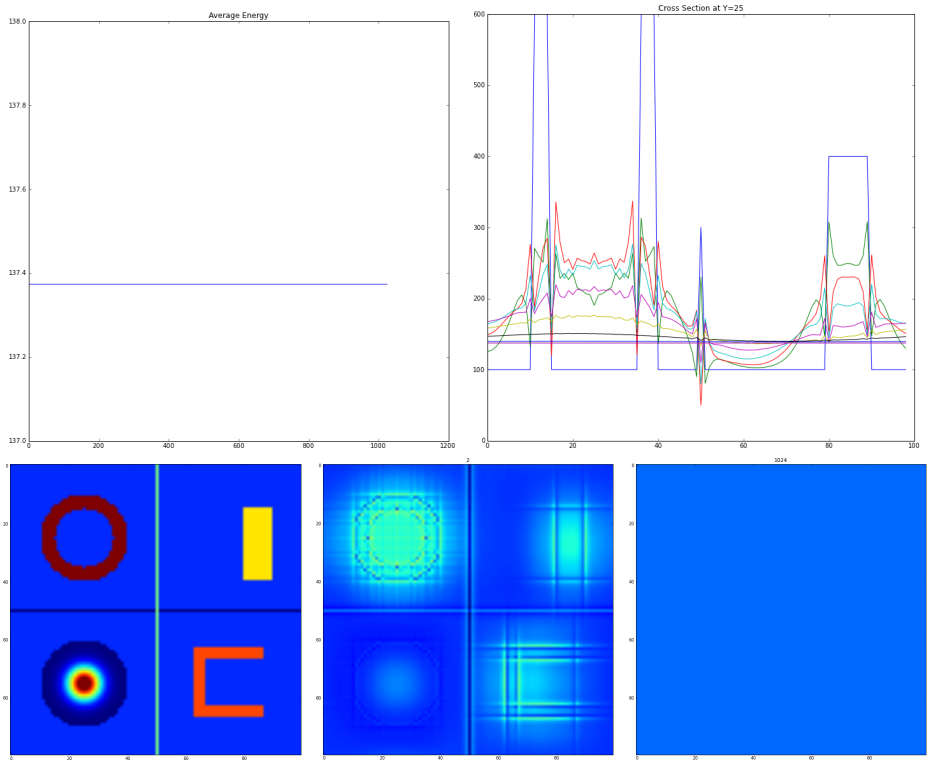


In addition we can simulate 1024 steps of a zero average system, which though not very realistic, still can be simulated by the CNM. This shows the error in more detail, but stays restrained to well under 10^{-10}, which is very good considering the system normally runs with average energies on the order of 100, so a signal to noise ratio of $1 : 10^{-10}$ is more than sufficient.



3.3 Unconditional Stability

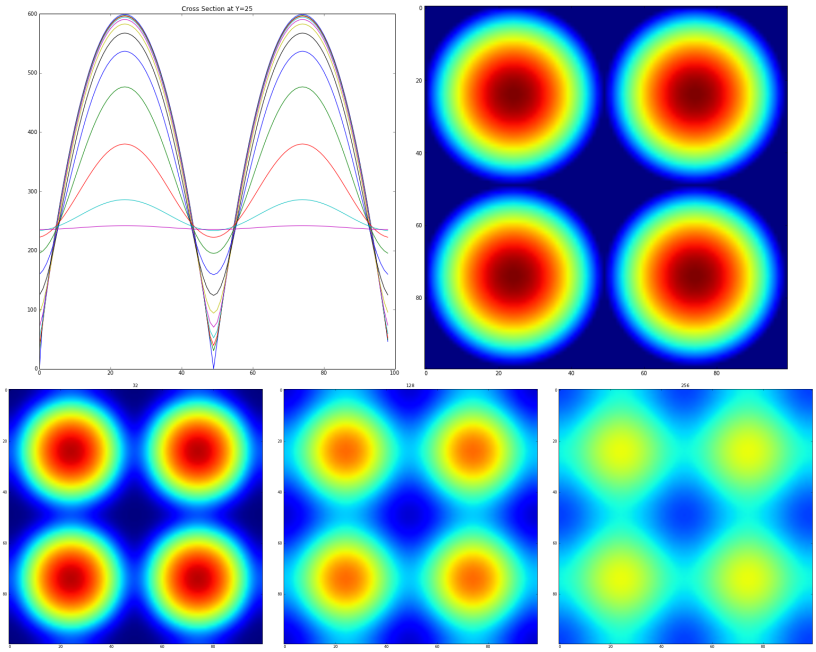
The CNM is supposedly unconditionally stable, which should allow for Δt of any size while maintaining stability, and hopefully energy conservation as well. To test we can run a 1024 step run with $\Delta t = 10$



Though we can see significant lack of accuracy from the cross section and heat map at $t = 20$, the system does stay stable, conservers energy, and even happens upon the correct equilibrium solution!

3.4 Visualization of Boundary Conditions

To help us visualize these boundary effects, let us consider a system of 4 paraboloids



We will discuss the evolution of a paraboloid later, but for now we can use it as a helpful example of the periodic boundary conditions of our system.

As you can see, rotational symmetry is broken due to the non-symmetric distribution of neighbors, resulting in an angled checker-board pattern. It should be noted that effect is not a computational error, but rather an artifact of the boundary conditions.

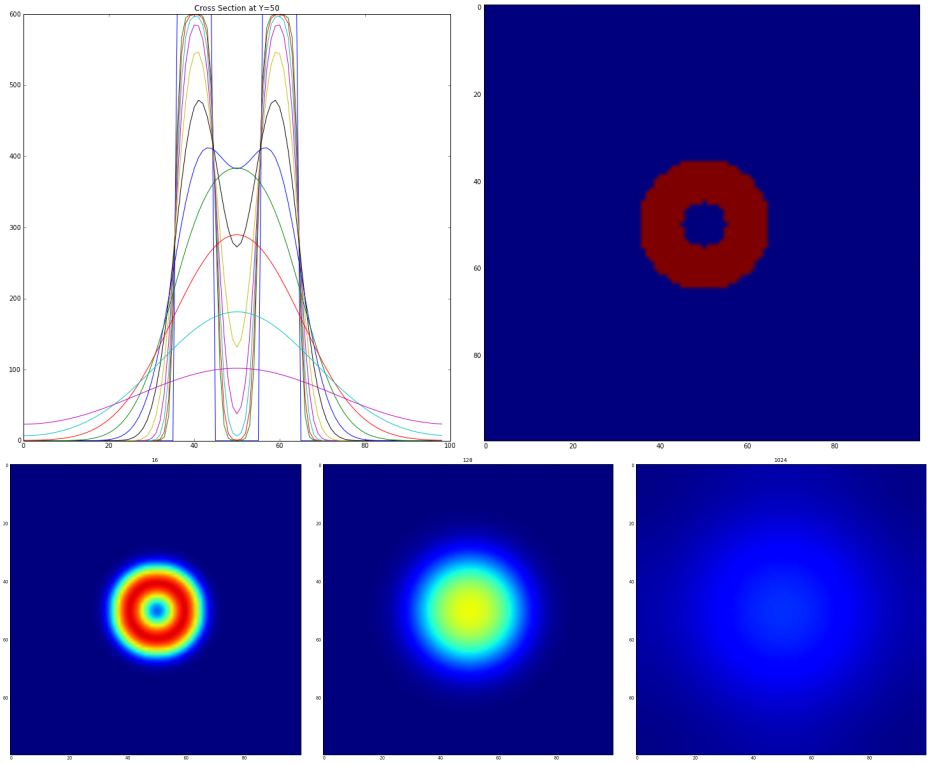
3.5 Testing Conclusion

By this point we have not only mathematically shown our method to be to the CNM, we have also shown that our implementation of it correctly satisfies 3 conditions of the CNM: Numeric accuracy, energy conservation, and unconditional stability. We will now work under the assumption that our method is sound and begin to characterize the time evolution of a few interesting initial conditions.

4 Case Studies

4.1 Small Ring

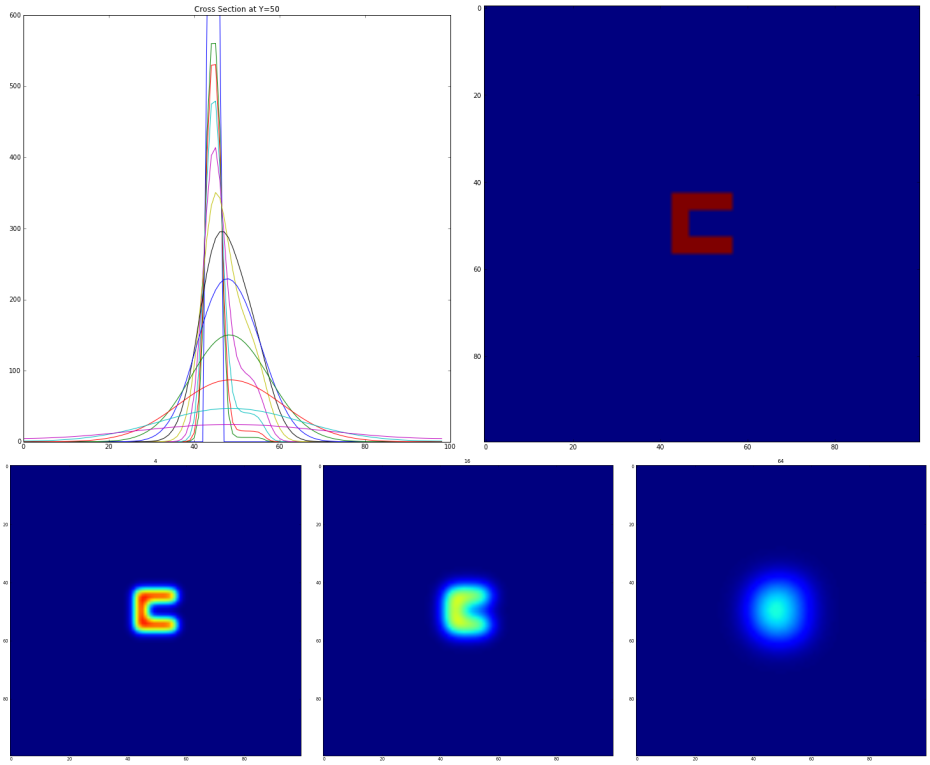
We have already covered the case of a delta function in our error analysis, so let us move on to a similar but more exciting case, a small hot ring.



The ring begins to cool much like we would have expected, keeping its circular shape, but then after 128 steps when $t \approx 30$, we see an interesting shift. The "twin peaks" we can the cross section begin to move towards each other, before merging and resembling the gaussian shape we would expect from a delta function. This makes sense because to a large enough approximation ($\Delta x \approx r$) a hot circle does resemble a delta function, so its not surprising to find that they have similar solutions after a reasonable amount of time has passed.

4.2 U-Shaped Disturbance

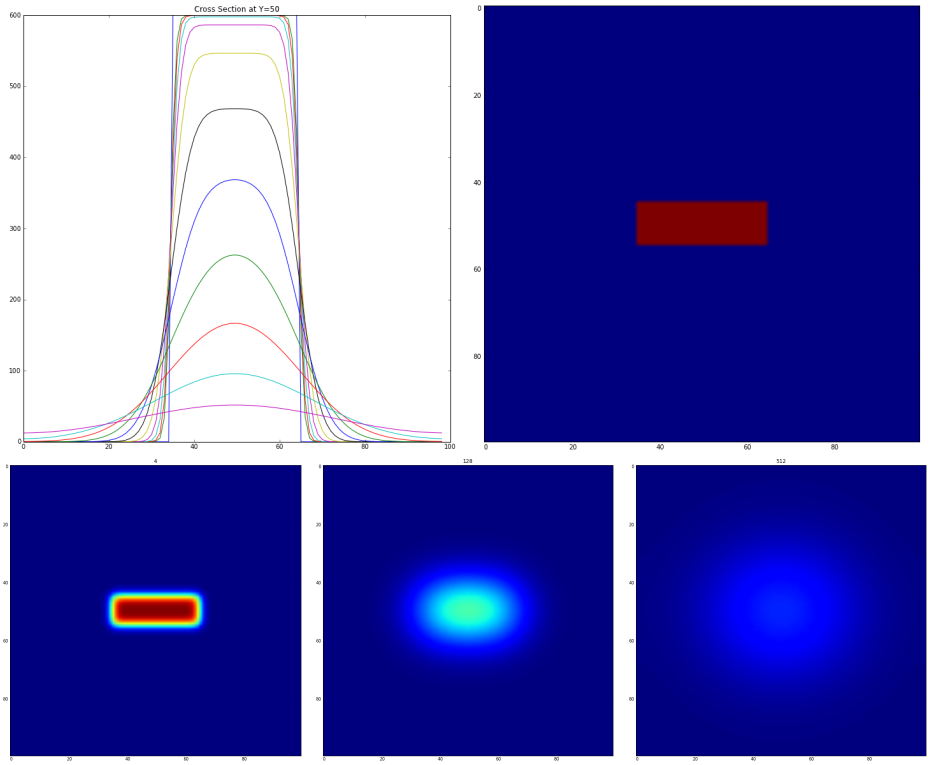
Out next case is that of a hot, collection of 3 rods in the shape of a U.



We can first see the hard edges round out on the U, giving it a more truly round U shape. We then begin to see "bay" left at the center of the U begin to heat much faster than the surroundings, similar to the heating of the inside of the circle. But eventually, like always the heat profile begins to resemble that of a gaussian, though this time it appears less symmetric, not doubt an artifact of its asymmetric initial condition.

4.3 Rods

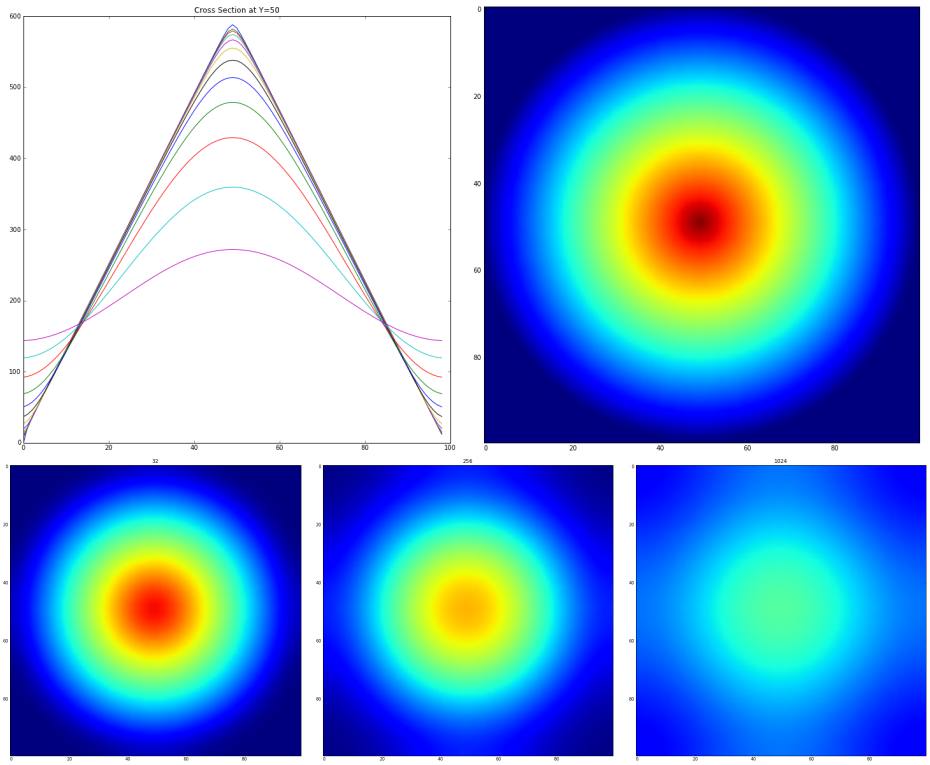
Now for a simple rod.



We again see the sharp edges very quickly cool and round out. This can be explained by the high inflection at these sharp edges resulting in a rapid cooling. The opposite effect can be noted on the interior, which is relatively flat and does not cool much until it begins to have a significant curve to it. This is a nice visual example of how the magnitude of the spacial inflection determines the rate of cooling, as indicated was indicated by the original heat equation.

4.4 Cone

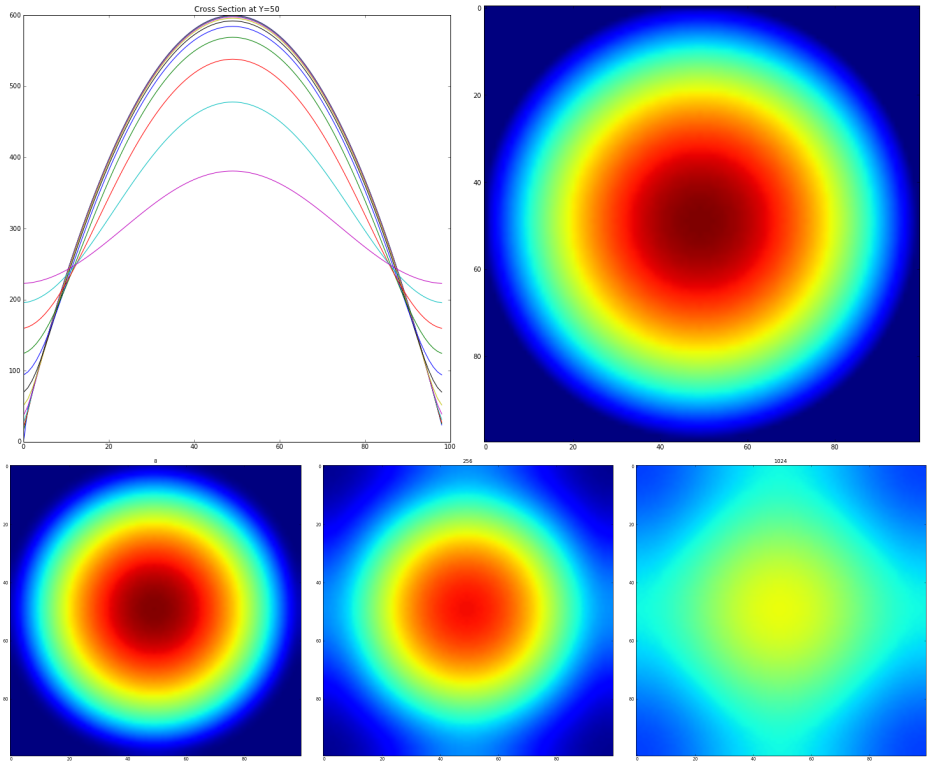
To further prove this point, we can consider the case of a cone, where initial the inflection is 0 everywhere except at the tip and edges.



As expected, we find the cone to actually be a rather stable shape, even though it is not isothermal. We see that the edges and tip are quick to change, while the sides of the cone stay rather stable. We can see from both the cross section and heat maps that the tip rapidly cools and the midsections remain relatively constant temperature for early t. This of course only last for a short while until the sides too eventually cool and the whole system moves towards the equilibrium state of equal temperature everywhere.

4.5 Paraboloid

Now to consider an example with constant inflection, the parabola.

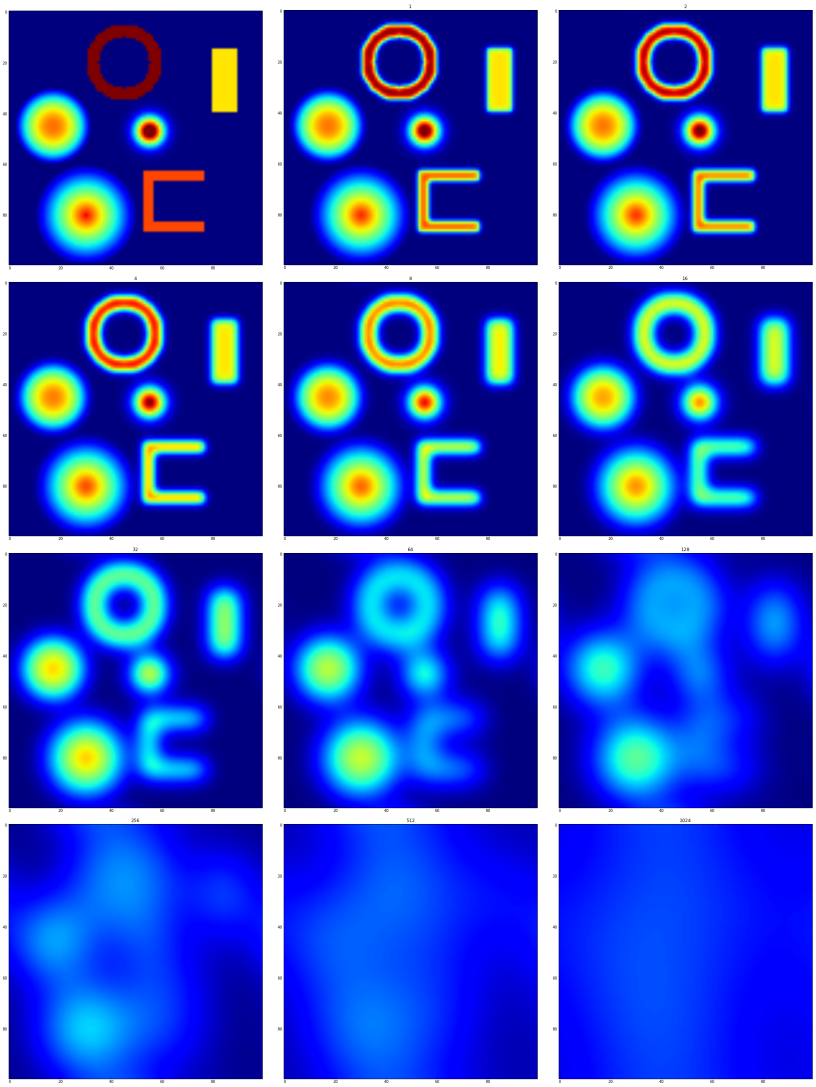


As we would expect, the system as a whole seems to cool a constant rate, with no one spot cooling significantly faster or slower. Note that the diamond shaped heat map on the final plot is due to the periodic boundary conditions of the system, not due to quantization error.

5 Conclusion

As a final visual treat, here is a full run of 1024 steps on a complex heat map. See if you can spot any heat features we may have discussed earlier!

I hope you have found this short introduction and explanation of the 2D Heat Equation modeled by the Crank-Nicolson method as interesting as I found the topic. If you have any questions, please feel free to ask away!



6 References

Many thanks to the following sources:

Wikipedia Articles:

-Heat Equation
http://en.wikipedia.org/wiki/Heat_equation

-Crank-Nicolson Method
http://en.wikipedia.org/wiki/Crank-Nicolson

T. Lakoba of the University of Vermont:
http://www.cems.uvm.edu/ tlakoba/math337/notes_15.pdf

Tristen Ursell of Cal Tech:
http://www.rpgroup.caltech.edu/courses/aph162/2006/Protocols/diffusion.pdf