Hi, everybody. Today I am going to tell you something about thermal conductivity.

In the computation of thermal conductivity, one of the easiest way one would think of is to impose a heat flux between a segment of a sample cell and determine the value of kappa by Fourier's Law. With the heat flux clearly known, this method of computation avoid the time-consuming process of converging the heat flux. But it uses only one pair of slabs during the simulation so a faster version may be to use all pairs of slab in between by imposing a sine function heat input. But how can we compute the thermal conduction with a non-linear temperature profile?

**Theory**

So here comes our theory:

By solving Peierls-Boltzmann equation, we can get an explicit expression of Fourier component of non-local thermal conductivity. Instead of transforming back into the real space, we remains in the reciprocal space.and the understanding of linear response theory tells us by taking the bulk limit where the wavelength vanishes to zero, the Fourier component of kappa goes to the limit of thermal conductivity in the real space.

**Liquid**

Firstly, we can test this algorithm on liquid.

Well, in the case of liquid. Because of the small mean free path, the Fourier component of kappa gives the exact result of thermal conductivity. And we can compare the results with calculation using Fourier's Law.

Those pictures show how the relative error changes as the system is running. The tests are conducted on a same system with the same initial input. From these two figures, we can clearly see the new algorithm converges faster than imposing heat input at the two end.

The second picture has a larger temperature variation so it converges much faster and it shows that the new algorithm can give a higher accuracy.

Well, before testing the performance of this algorithm in the case of crystal, we can next reivew on the theory that appears in the first two slides.

To get a theoretical extrapolation for the simulation, we apply our theory in the simplest case of Debye model. While in the spirit of Debye model, we not only have a constant group velocity, but also have a simplified mean free path dependence on the frequency of phonons. Then we can illustrate how k(q) behaves with different wavelength of phonon.

Here we have basically two methods of dealing with the formula here. In the an infinte crystal, we do the integral over the Debye sphere. While in the real model of supercell, we sum up over all wave vectors in the Brillouin Zone.

We can see little difference between them.

**Crystal**

When applying this new method to the LJ crytal of argon, we can see a fairly different picture from liquids---- Here, the kappa(q) substantially depends on the value of wavelength q. And from theory prediction on the slide, we can see that no matter how the mean free path of the phonon behaves with the change of q, the Fourier component of kappa will approach the real thermal conduction predicted by Debye model. This is basically protected by the math when we do the integral in the case of q equals 0.

When combining this theory with data from stimulation, we can see that the value of kappa(a) does not change a lot when the wavelength is small enough. This means that we don’t have to increase the length too much to get a close result.