Modeling mixtures of different mass ultracold atoms in an optical lattice: a CAP on the ERDC XT4 (Jade)

J. K. Freericks

Department of Physics

Georgetown University

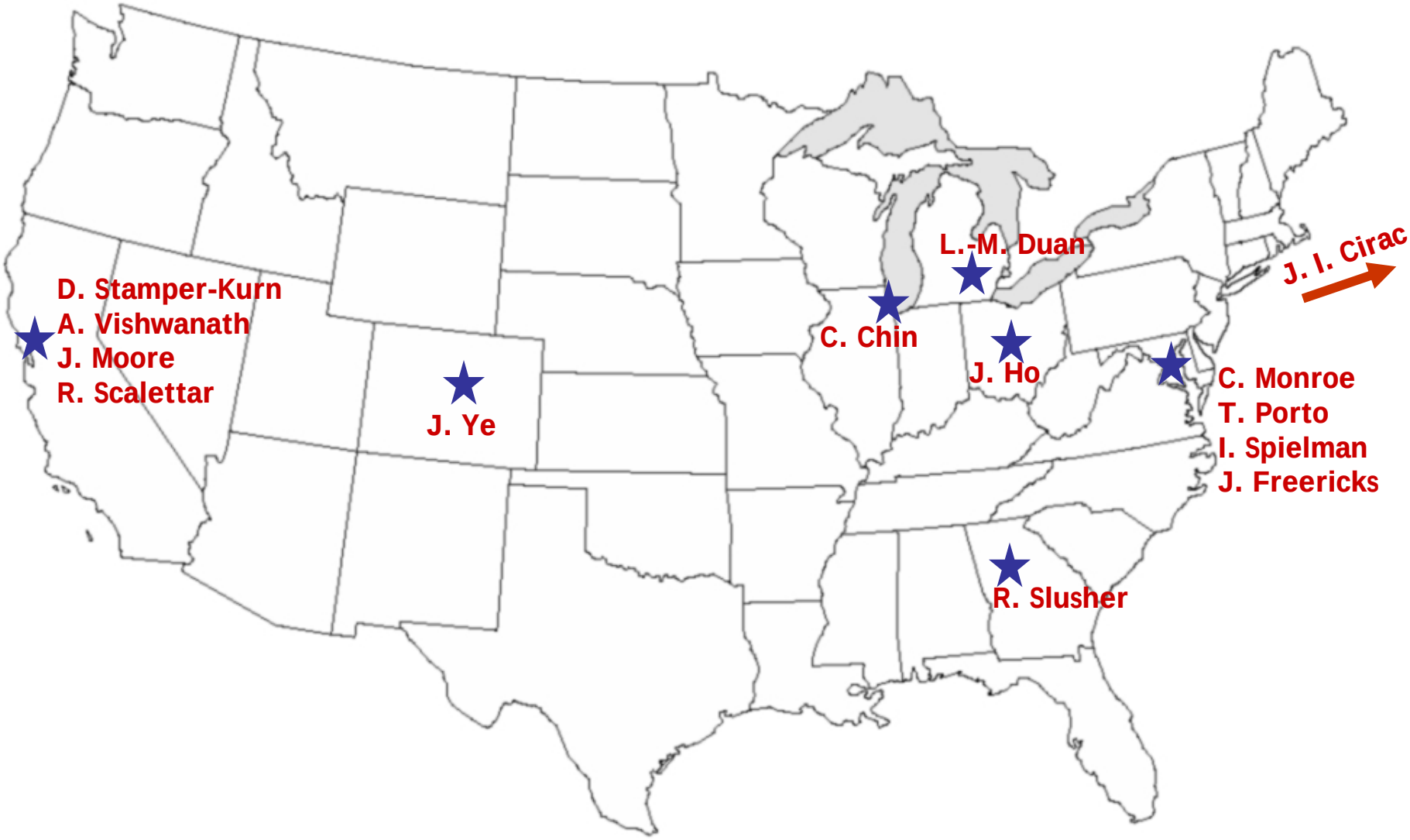
Optical Lattice Emulator

- DARPA is engaged in a program to create an analog quantum computer that can simulate models of strongly interacting systems in condensed matter physics.
- The program could ultimately lead to the ability to design, test, and create artificial (quantum-engineered) materials with tailor-made properties for various applications within the military.

Our experimental systems

- Expt 1: trapped ions interacting with lasers to simulate interacting quantum spins.
- Expt 2: neutral (Bosonic) atoms on an optical lattice that undergo a superfluid-insulator transition.
- Expt. 3: neutral (Bosonic) atoms that create magnetic crystalline phases.
- Expt 4: dipolar molecules created from different mass atoms and interacting in a lattice.

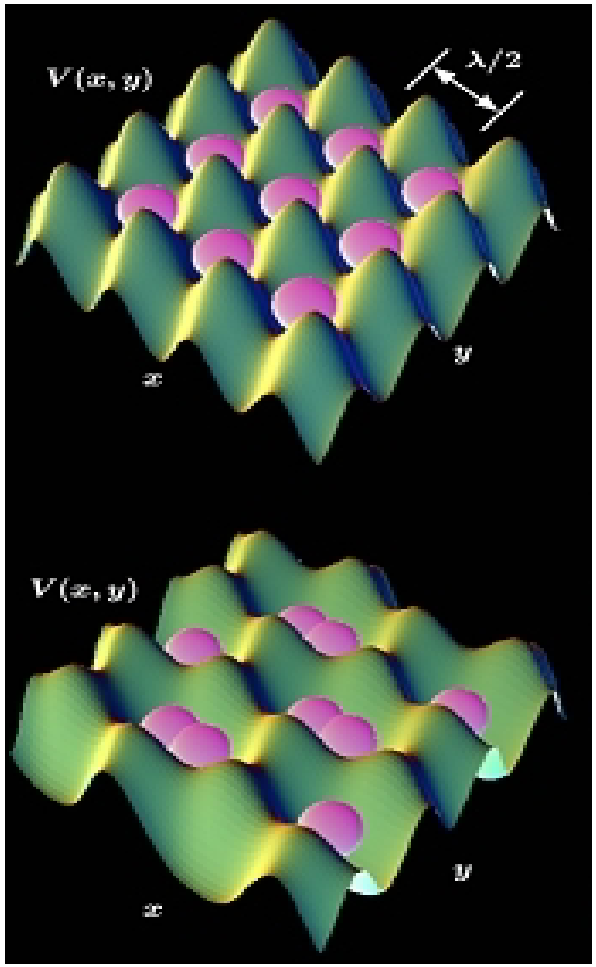
Location of our team members



Simulations of quantum mechanics on two complementary AMO platforms:

Ion Traps

Optical lattices



Role of theory in the OLE project

(1) Accurate calculation of phase diagrams for benchmarking

(2) Postprocessing of OLE data to find homogeneous (bulk) phase diagrams

Mixtures of different mass neutral atoms in an optical lattice

System modeled by the OLE

- The light (Fermionic) atoms hop from one site to a nearest neighbor site with a quantum-mechanical tunneling probability that is fast relative to the time-scale for the experiment.
- The heavy (Fermionic) atoms hop from site to site with a quantum-mechanical tunneling probability that is slow relative to the time scale for the experiment.
- The two atoms interact with each other when they sit on the same lattice site; this is described by the so-called Falicov-Kimball model.

Inhomogeneous dynamical mean-field theory

Many-body physics approach

We employ a Green's function-based approach to solve the quantum-mechanical problem.

It is based on dynamical mean-field theory, which assumes the self-energy is local, but can vary from site to site.

The formalism can be solved with a massively parallel approach, and is well suited for high performance computing.

Computational elements

There are two main computational elements to the IDMFT algorithm: (i) solving the Dyson equation and (ii) determining the local density of the light and heavy atoms.

Solving the Dyson equation requires inverting an NxN matrix (N is the number of lattice sites) for each Matsubara frequency used in the calculation. This parallelizes by sending the calculation for each frequency to a different slave node.

Solving for the local densities requires summing the Green's function over all Matsubara frequencies for each lattice site and evaluating infinite products of expressions derived from the Green's functions for each lattice site. This parallelizes by sending calculations for each site to a different node.

The communications are minimal, because they require sending the self-energy vector or the Green's function vector to each slave node.

Efficient implementation

Matrix inversions are computed using LAPACK and BLAS routines tuned for the specific processor available in the machine.

The number of Matsubara frequencies required is reduced by an order of magnitude by employing high frequency sum rules which allow for the large frequency tails of the summations or the infinite products to be evaluated exactly.

Once the fillings and chemical potentials are known from the imaginary-axis calculations, real-axis calculations are then performed to determine other properties, like the entropy distribution.

Challenges

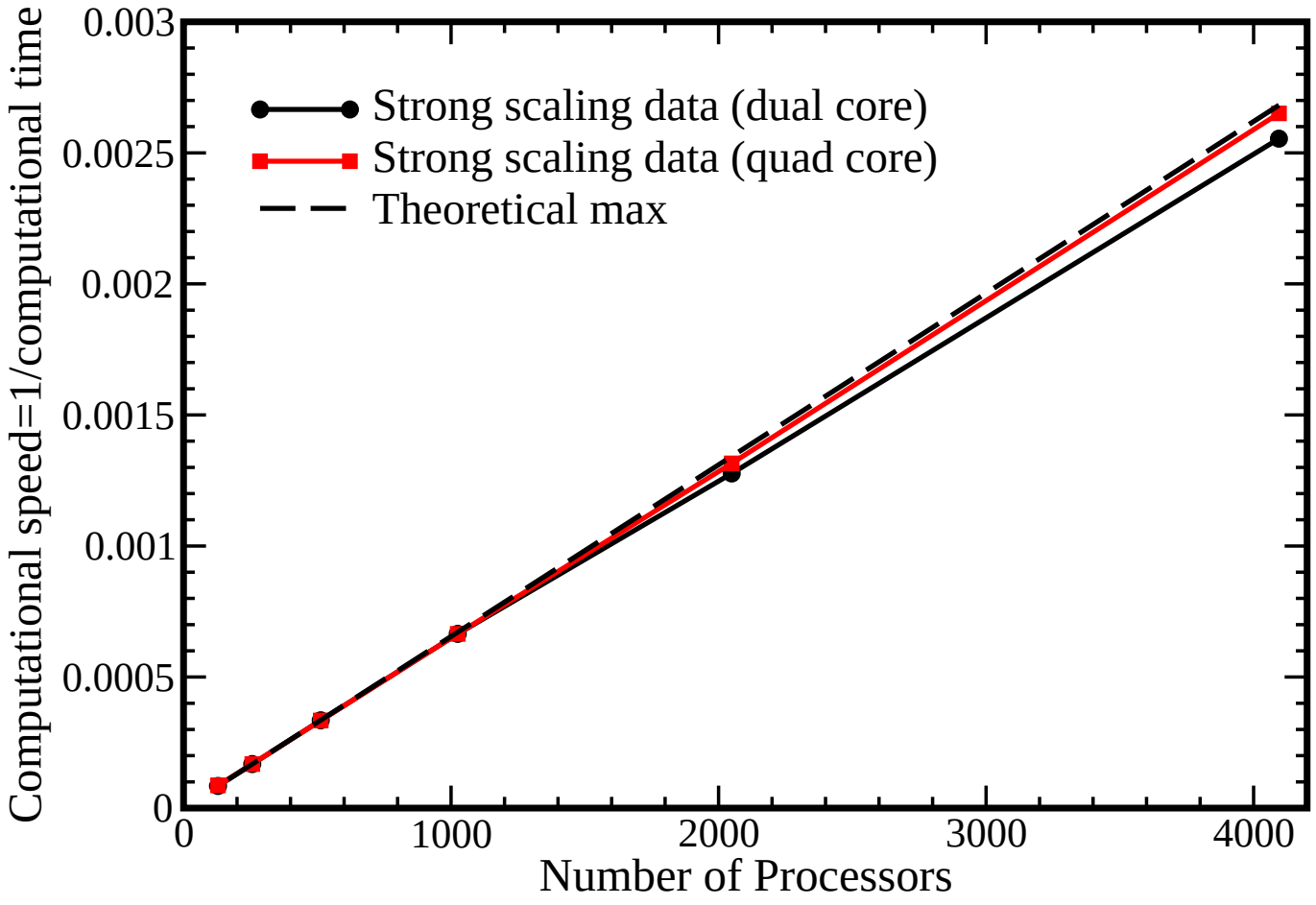
The calculations become difficult at low temperature, where the system tends to phase separate. In this regime, we may need many thousands of iterations of the IDMFT equations, and we may need to run for many values of the chemical potentials until we determine the correct values for the target total numbers of heavy and light particles.

Jade configuration during CAP

- Jade was initially configures with about 2100 dual core 1.8GHz processors, each capable of two operations per clock cycle or 3.6 Gflops per processor.
- After it was rebuilt, it had about 2100 quad core 2.1 GHz processors, each capable of two operations per cycle or 4.2 Gflops per processor.

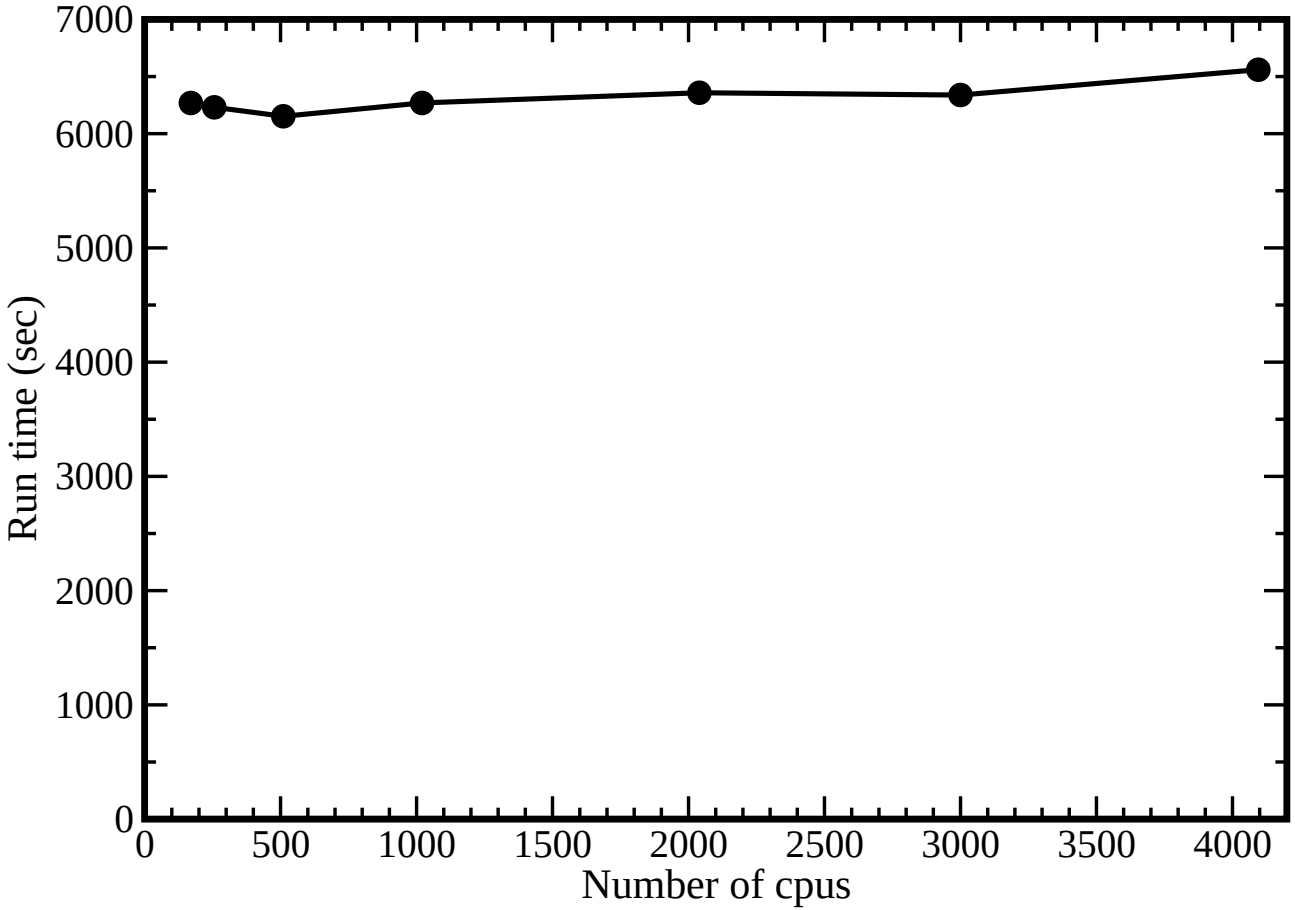
Scaling runs for the code

- Using the initial configuration, we ran a series of weak and strong scaling runs to establish how the codes functioned, to tune them to the machine, and to compare different libraries for efficiency.
- In addition to straightforward timing runs, we also used the PAPI suite to determine the number of Gflops per processor and find out what percentage of peak speed the code ran at.
- The scaling runs were quickly retested with the new and improved jade after the processor upgrade. Our scaling and efficiency benchmarks were excellent in essentially all aspects.



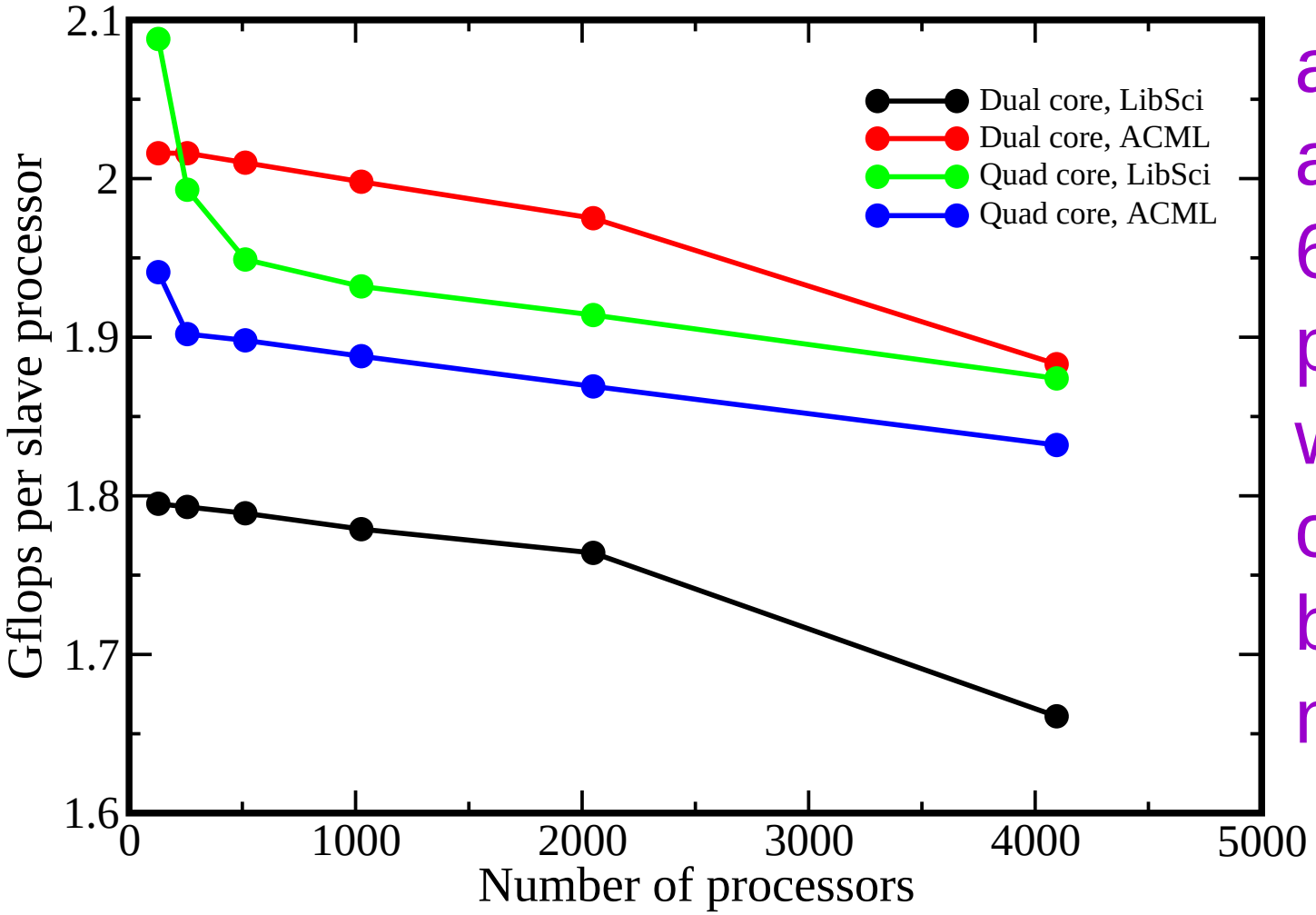
achieve
rox-
tely
% of
ar
ling for
inal
e and
% for
/ jade!

Weak scaling



'eak
:aling
:sted only
ı original
de) was
most
:rfect up
4000
ocs.

Efficiency



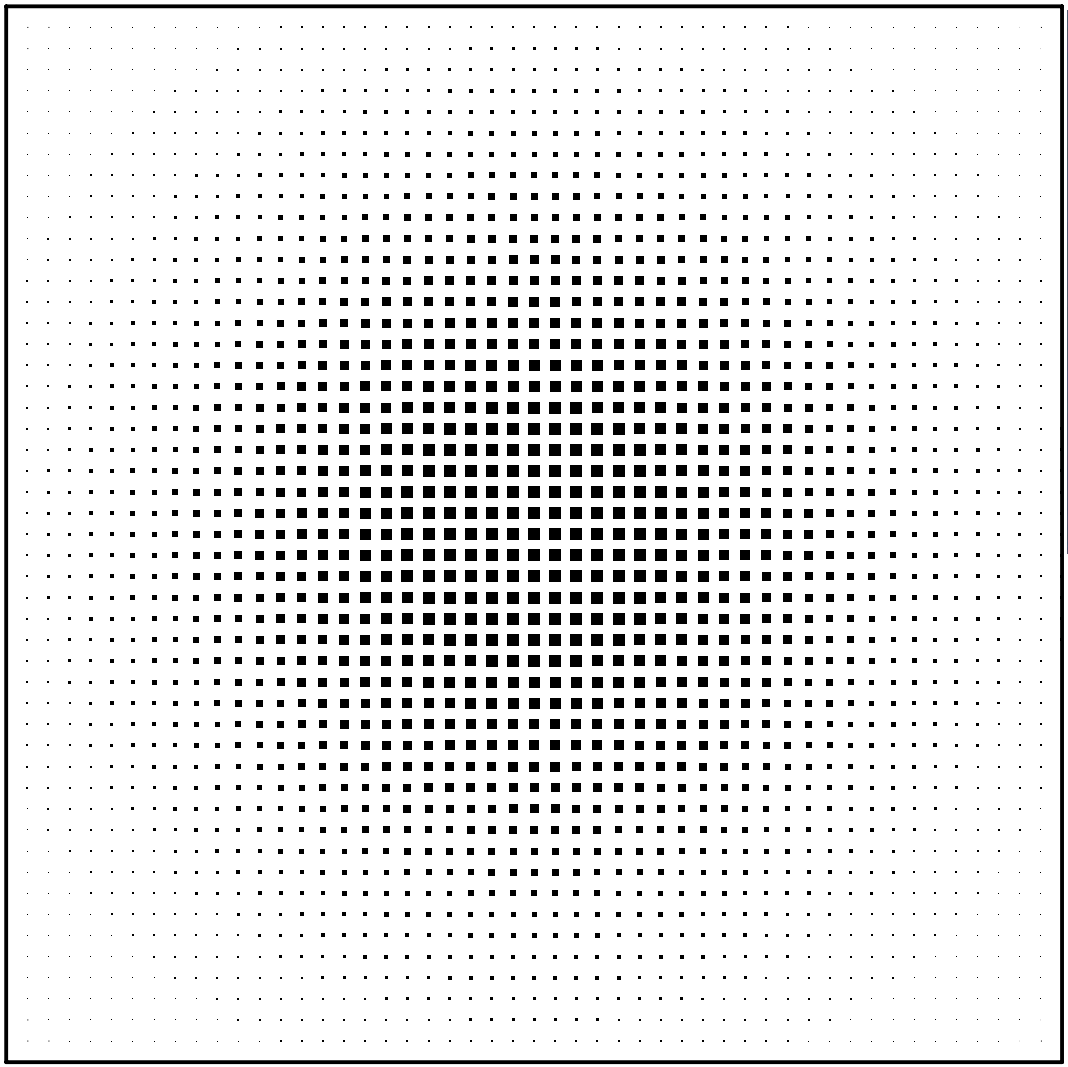
We achieved about 40--60% of peak performance with this code for both old and new jade.

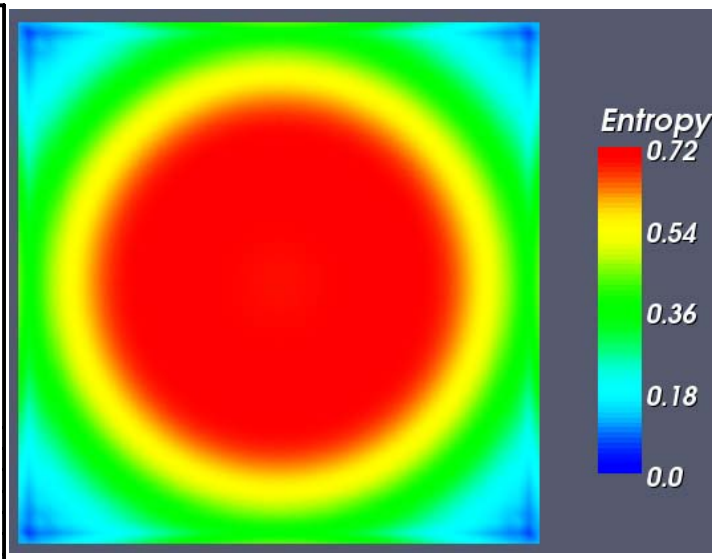
Results

Cases examined

- In cold atom experiments, the atoms are confined by a harmonic trap which pushes them toward the center of the lattice. We work with a 51x51 square lattice.
- The trap for the heavy atoms is fixed at a characteristic length of 30 lattice sites.
- The trap for the light atoms is varied from 30 to 12.9 lattice sites.

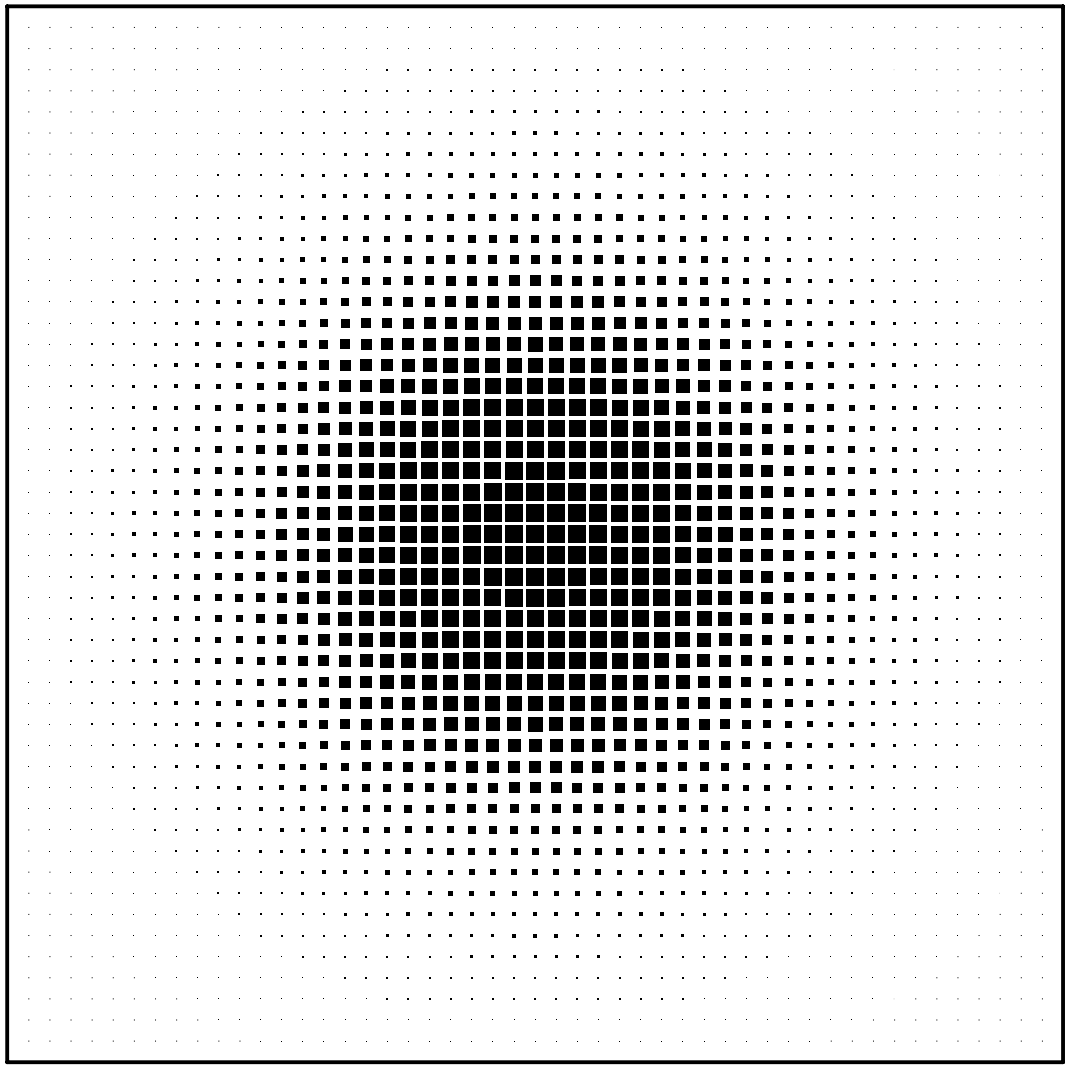
R=30, T=0.2

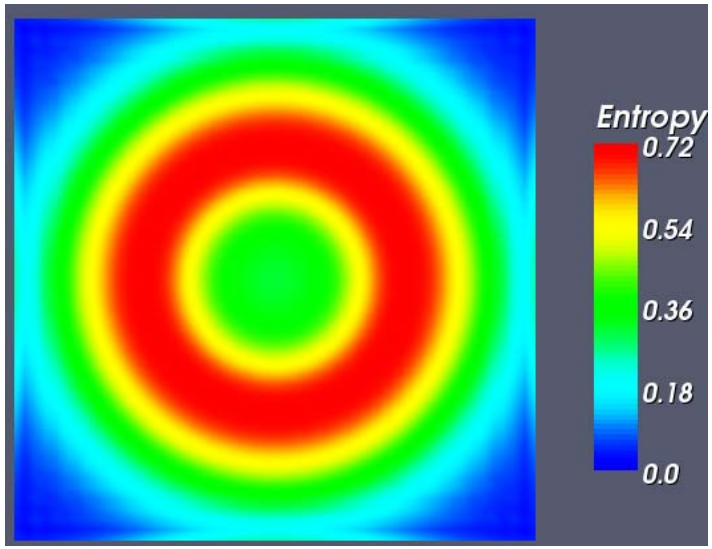




No ordering yet.

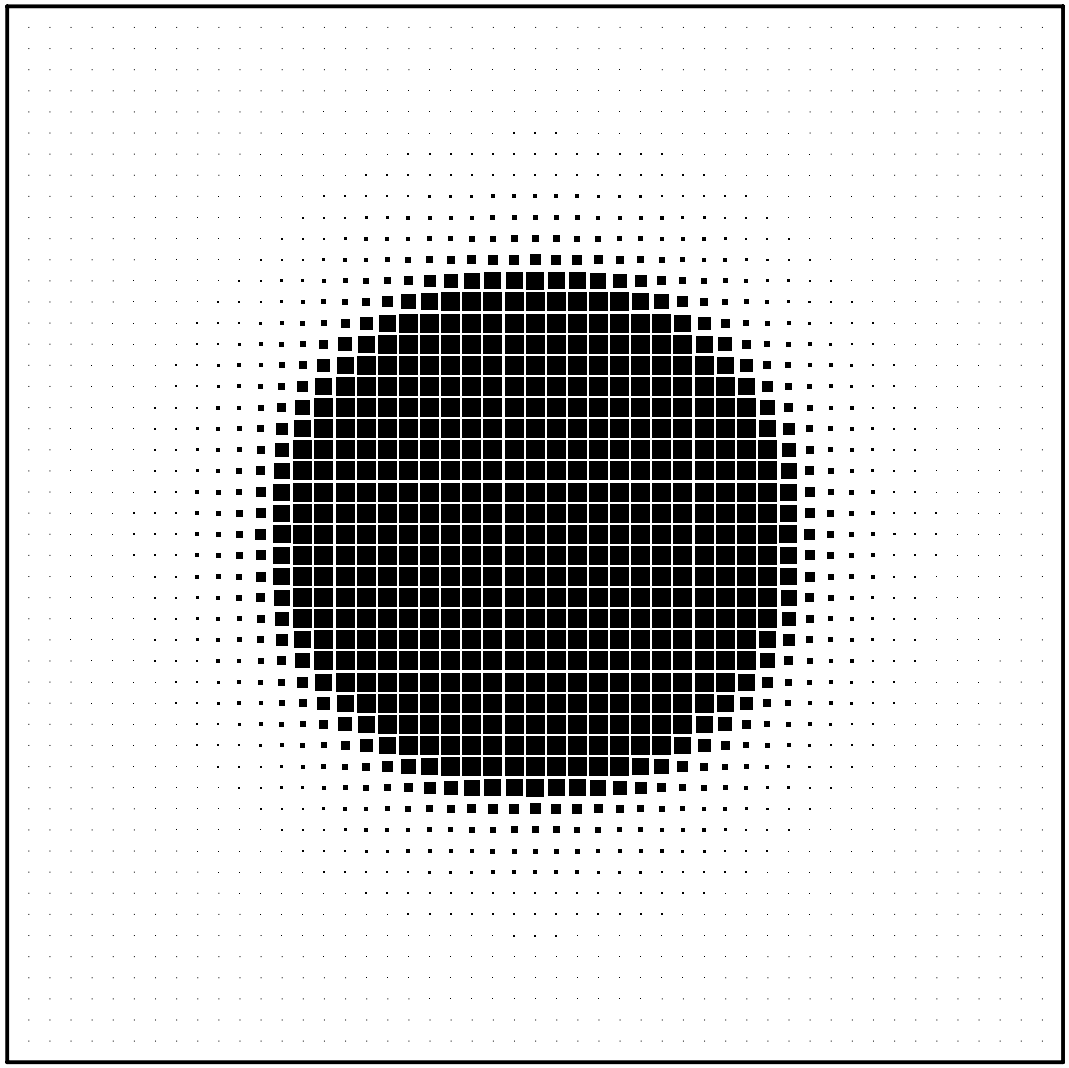
R=30, T=0.125

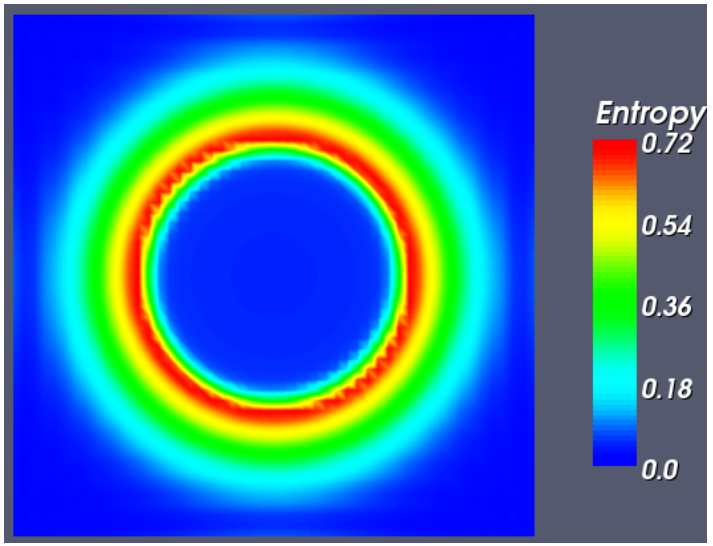




Ordering begins.

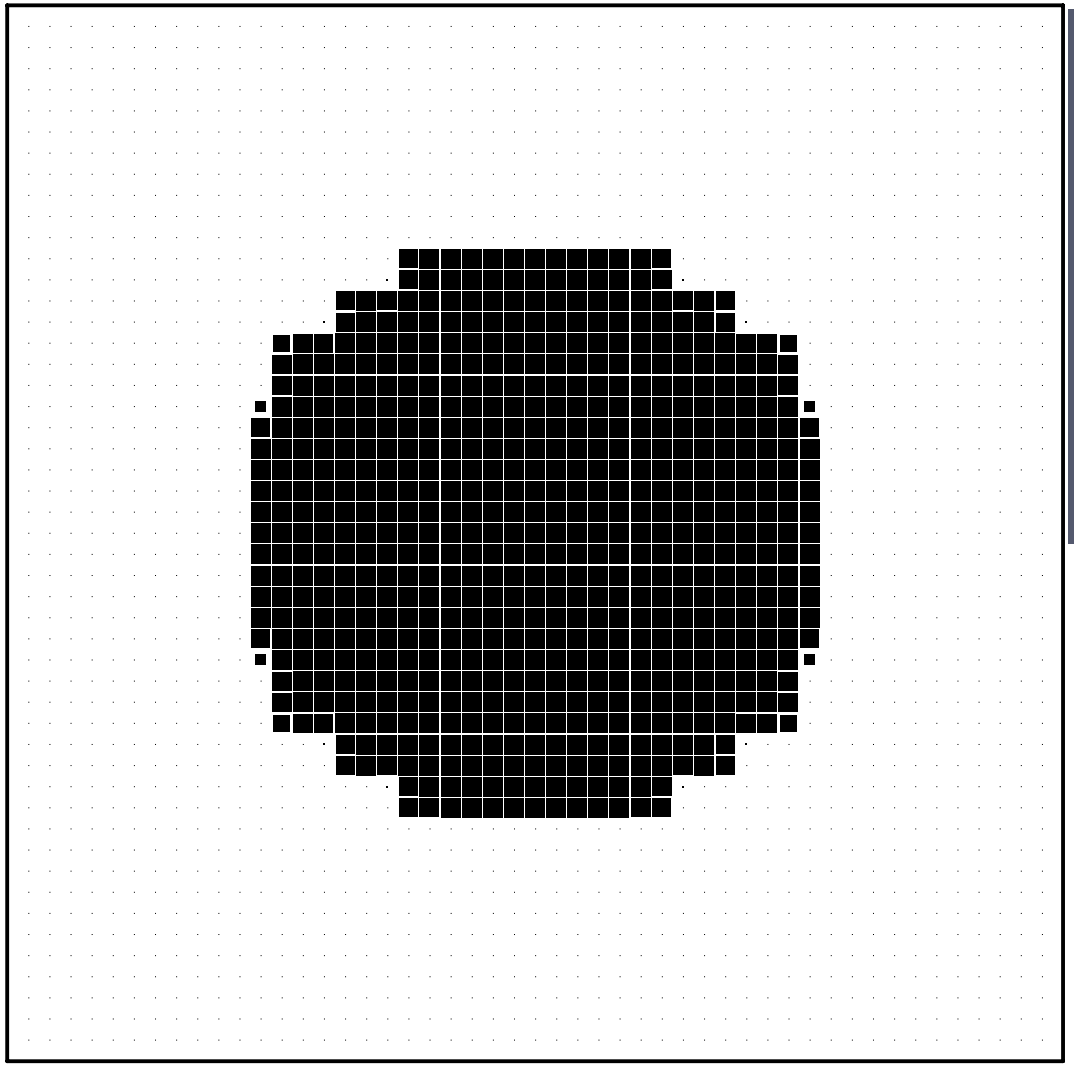
R=30, T=0.075

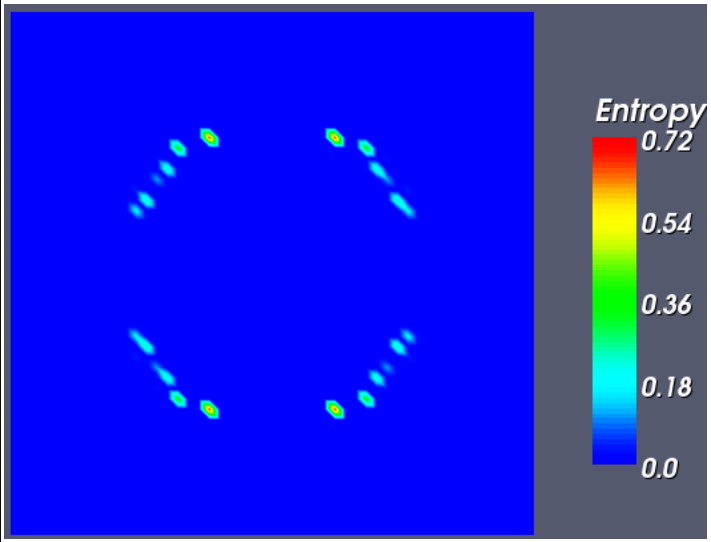




Ordering deepens.

R=30, T=0.01



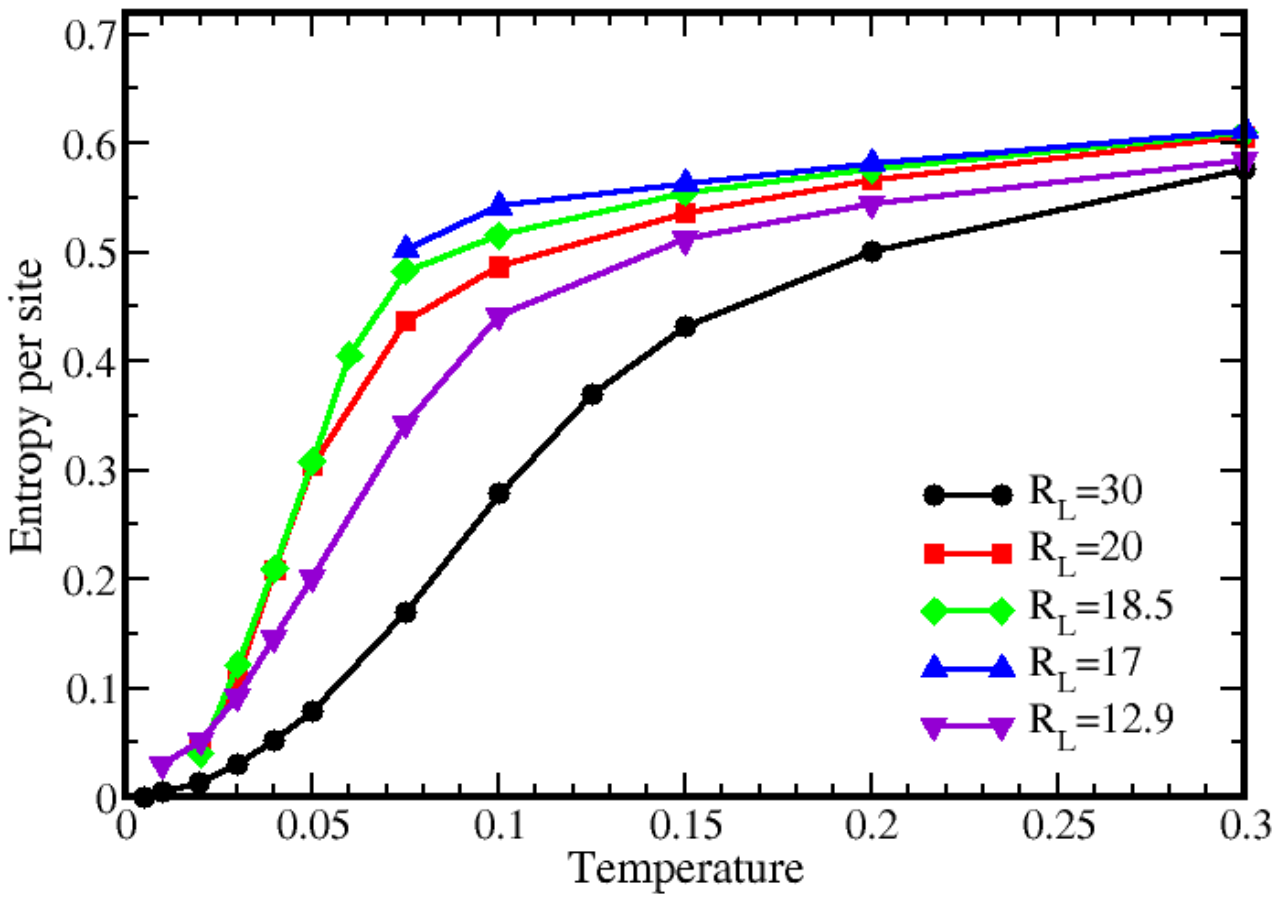


The system shows well-developed facets.

Applications

- As the system orders, the entropy is sharply reduced.
- The ordered patterns develop at particular temperatures. Signatures of specific patterns could be seen in Bragg diffraction and serve as a thermometer within the optical lattice. Finding good thermometers at these low temperatures is one of the grand challenges in the field.

Entropy curves and cooling



The entropy vs temperature curves show there might be a chance to cool if one can perform both adiabatic and isothermal processes for a “heat engine”.

Conclusions

- Described some HPC-based calculations for the DARPA OLE project
- Our codes are both highly efficient and scale well up to many thousands of processors.
- Experiments on mixtures are expected to be done within one to two year's time. This work is helping narrow the parameter space for the experimentalists.
- Results from this work may be able to help develop low-T thermometry within a lattice or may show how to cool the system within the lattice.