

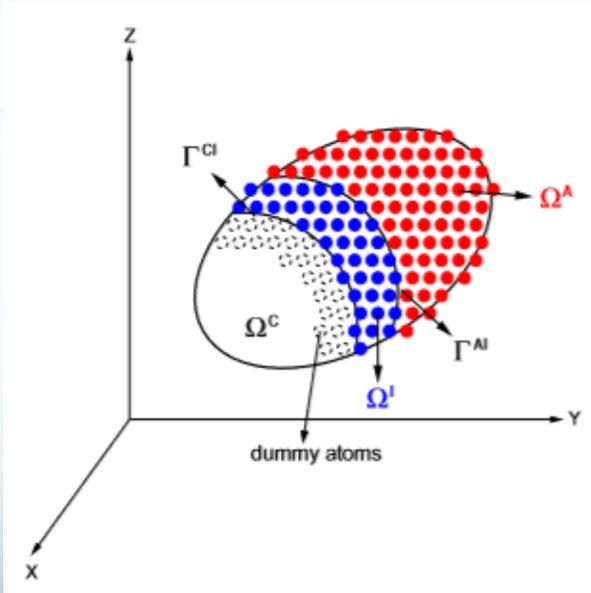
# A Concurrent Atomistic Continuum (CAC) Method in LAMMPS

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August 14, 2019

# Concurrent Multiscale Methods

Existing Multiscale Methodologies lack predictive power in the realm of dynamic simulation due to restrictive interface treatments, different representations of governing laws, constitutive relations, or even just their implementations as codes with limited parallel capabilities.



- A simple illustration of a Multiscale model with three regions (atomic, coarse grained, and the interface between them) is shown.
- Many multiscale methods have a separate governing law defined for each of these regions; although for many the interface law is just a weighted sum of two different governing equations.
- The coarse grained region is typically populated by Finite Elements as part of a numerical solution.

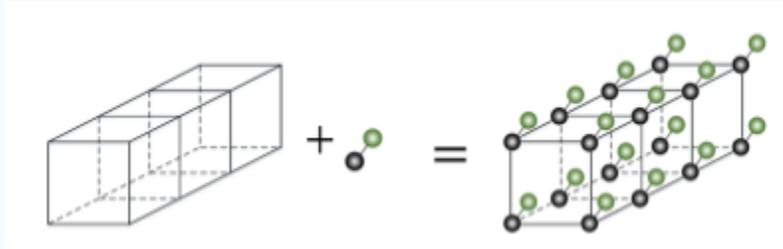
Fish, Jacob, et al. "Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force."

# Motivations and Objectives

- Establish and formulate a Concurrent Atomistic Continuum (CAC) multiscale methodology for massive parallel computing to enable simulation of dynamically coupled mechanical and thermal transport behavior at the mesoscale. The strengths of this method are its ability to provide the following with no additional constitutive treatment:
  - 1) seamless atomic to continuum coupling; one governing equation.
  - 2) a coarse grained nucleation and propagation of lattice defects.
  - 3) accurate long wavelength propagation in the coarse grained region.
- Establish the CAC method in LAMMPS; an open-source object oriented framework that will enable community use and development.

# The CAC Formalism

The CAC methodology is based on a multiscale representation of conservation laws, reformulated as an extension of the IK (Irving-Kirkwood) statistical mechanical theory of transport processes for single-component systems to general polyatomic crystalline materials. It only assumes the smoothness of unit cell deformation while retaining the predictive power of interatomic interaction; thus removing many of the predictive barriers to multiscale methods.



One marked distinction with all other multiscale methods is the use of a concurrent two-level materials description by including internal degrees of freedom into the unit cell deformation. The resulting methodology affords predictive power in the realms of phonon and defect analysis that approximates that of MD.

Chen, Y. Reformulation of microscopic balance equations for multiscale materials modeling.

The Journal of Chemical Physics 130, 134706, (2009).

# LAMMPS CAC

## The Governing Equation

The reformulated conservation equation of momentum can be expressed in terms of internal force density and kinetic temperature :

$$\rho^{\alpha} \mathbf{u}^{\alpha} + \frac{\gamma^{\alpha} k_B}{\Delta V} \nabla_x T = \mathbf{f}_{\text{int}}^{\alpha} + \mathbf{f}_{\text{ext}}^{\alpha}, \quad \alpha=1, 2, \dots, \nu$$

The equation is then then discretized and solved using the Galerkin method typically used in FEA:

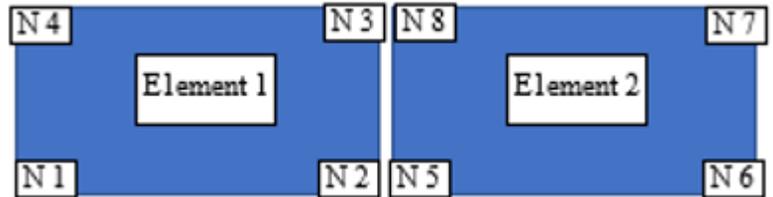
$$\int_{\Omega(x)} \Phi_{\eta}(x) \left( \rho^{\alpha} \mathbf{u}^{\alpha}(x) - \mathbf{f}_{\text{int}}^{\alpha}(x) - \mathbf{f}_T^{\alpha}(x) + \mathbf{f}_{\text{ext}}^{\alpha} \right) dV_x = 0$$

where  $\Phi_{\eta}$  are the basis functions used to interpolate the displacement field for each internal degree of freedom (atom in the unit cell). The thermal forces are considered negligible for current applications and omitted.

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## The FEA Solution

- We solve CAC's governing equation using the Galerkin Method of FEA. Note that the governing equation admits discontinuous interpolation fields.



$$\mathbf{M}_\alpha \ddot{\mathbf{U}}_\alpha = \mathbf{F}_\alpha$$

$$\mathbf{M}_\alpha = \int_{V_X} \rho_\alpha(\mathbf{X}) \begin{pmatrix} N_1(\mathbf{X})N_1(\mathbf{X}) & \dots & N_1(\mathbf{X})N_n(\mathbf{X}) \\ \vdots & \ddots & \vdots \\ N_n(\mathbf{X})N_1(\mathbf{X}) & \dots & N_n(\mathbf{X})N_n(\mathbf{X}) \end{pmatrix} dV_X$$

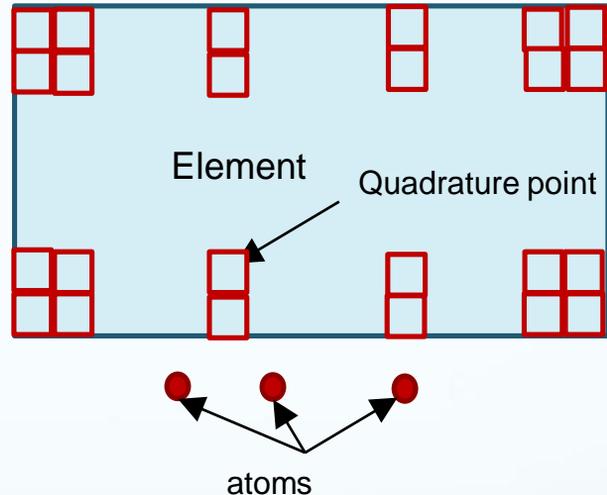
$$\mathbf{F}_\alpha = \int_{V_X} \begin{pmatrix} \mathbf{f}_\alpha(\mathbf{X})N_1(\mathbf{X}) \\ \vdots \\ \mathbf{f}_\alpha(\mathbf{X})N_n(\mathbf{X}) \end{pmatrix} dV_X$$

- One way to exploit this is by using an unconnected set of elements. This makes the matrix equation block diagonal with one block for every element in the system. The major task remaining is to compute forces.

# LAMMPS CAC Algorithm

## Computing Force Density

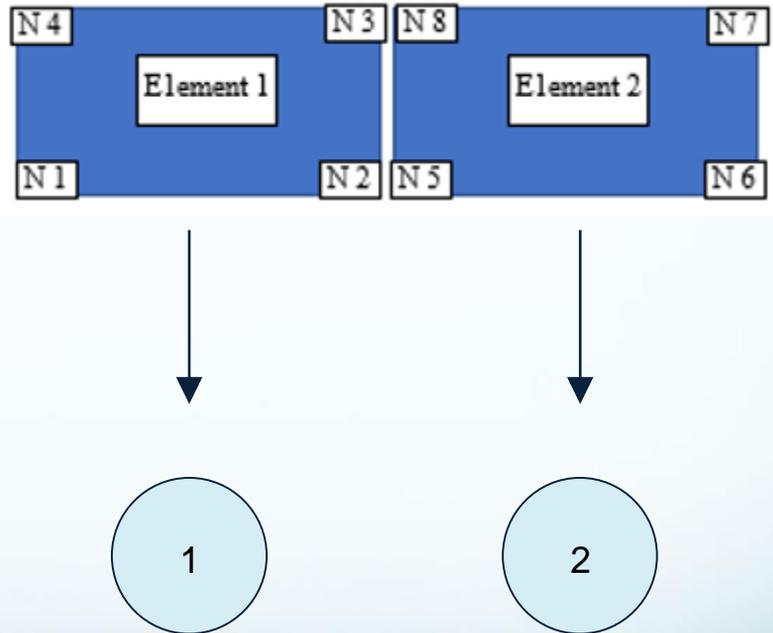
- The CAC code computes the Force vector required to update by using Gaussian Quadrature over the coarse-grained domain and Dirac pulses over the atomic (which results in the simple discrete force calculation of MD for particles).
- The forces at each quadrature point in an element, required by the quadrature rule, are computed very similarly to how they would be computed for an atom.
- This is enabled by defining the force density as a unit cell average (the shape function is an approximation of this tiling of cell averages)



# LAMMPS CAC Algorithm

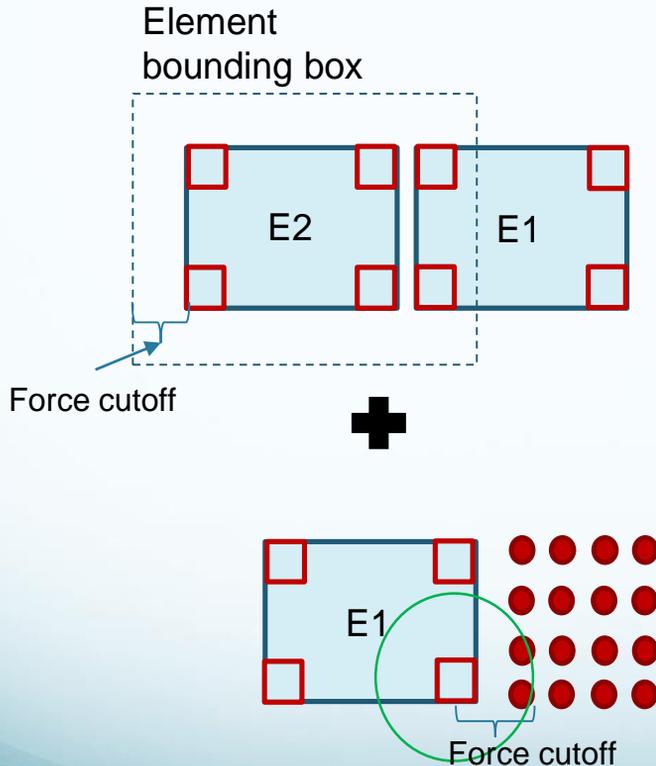
## FEA in LAMMPS

- 1) LAMMPS is parallelized for solutions of systems involving many particles coupled by non-local interactions
- 2) LAMMPS is object oriented to allow the definition of the FEA Elements as particles with properties.
- 3) The properties of adjacent elements can be communicated in the same fashion that LAMMPS communicates particle information



# LAMMPS CAC Algorithm

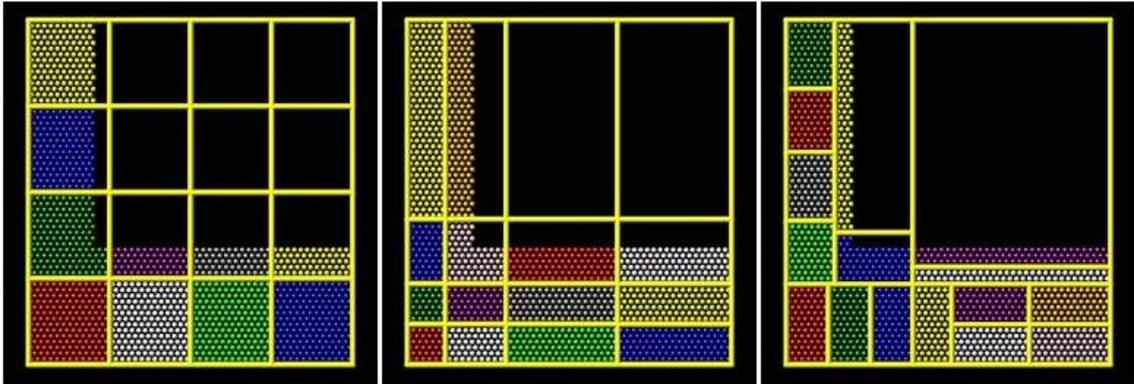
## The Neighbor-listing Process



- The computation of the non-local forces for each atom and finite element defined in the model requires obtaining knowledge about surrounding atoms and elements that are relevant to the force cutoff radius.
- To accommodate this need one can define the neighbor lists (containing finite element and atom indices) for both quadrature points and atoms.
- An element is considered relevant to the list if a bounding box expanded by the cutoff radius overlaps with a quadrature point or atom.

# LAMMPS CAC Optimization

## Non-Uniform Spatial Decomposition

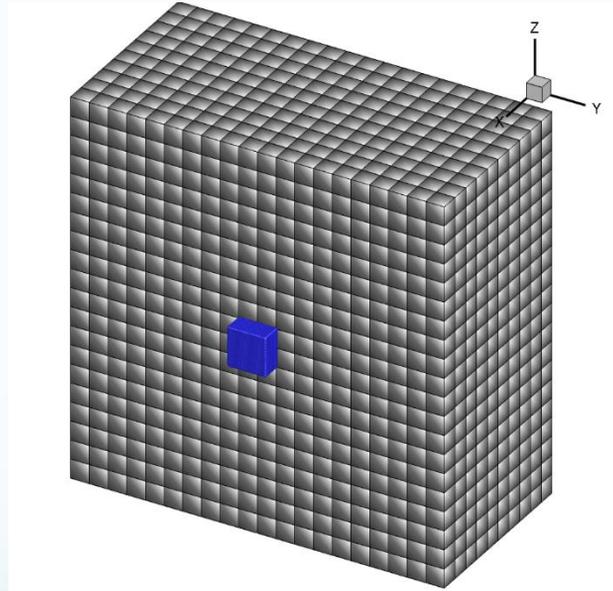


- The typical spatial decomposition algorithm utilized in LAMMPS for Molecular dynamics is very inefficient for systems containing finite elements with multiple length scales
- However, LAMMPS is also equipped with a non-uniform spatial decomposition algorithm capable of balancing models with differing resolution scales, the rcb (recursive coordinate bisection) algorithm.

# LAMMPS CAC Algorithm

## Scalable Multiscale Simulation

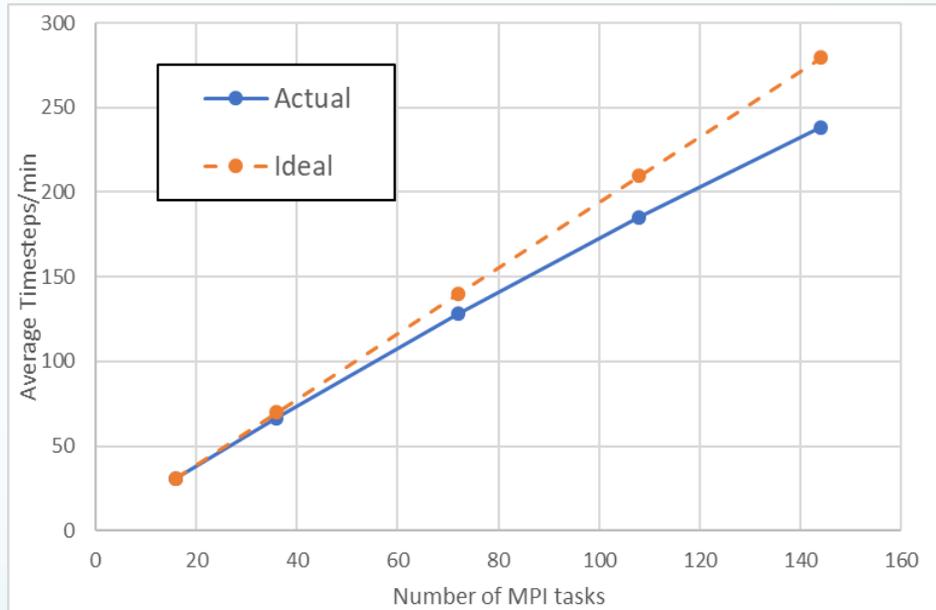
- As a simple benchmark of the algorithm a Copper Cube with two materials resolutions is relaxed for several picoseconds.
- The middle of the cube is composed of atoms; shown here via a cross section of the cube. The rest is composed of finite elements.
- Two sizes of this cube (one with eight times the content) were simulated.



# LAMMPS CAC Algorithm

## Scalable Multiscale Simulation

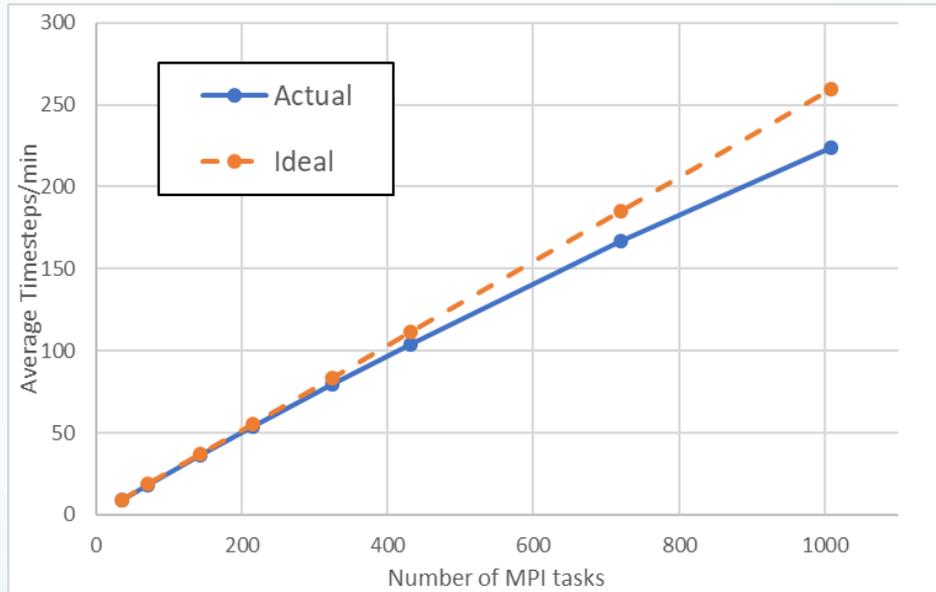
- The performance results for the relaxation of the Copper Cube.
- The Ideal line is an extrapolation from the first data point
- Parallel Efficiency starts to decline as this model becomes sparsely decomposed.



# LAMMPS CAC Algorithm

## Scalable Multiscale Simulation

- The performance results for a larger Copper Cube model (with 8 times the computational weight in atoms and elements).
- The Parallel Efficiency declines similarly at 8 times the task count of the smaller mode
- Provides reassurance that the efficiency scales with the average weight per task.

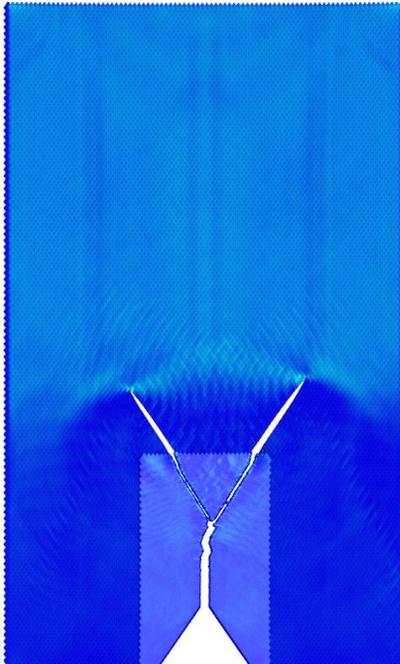


Note that this axis spans about 8 times more MPI tasks than the previous plot

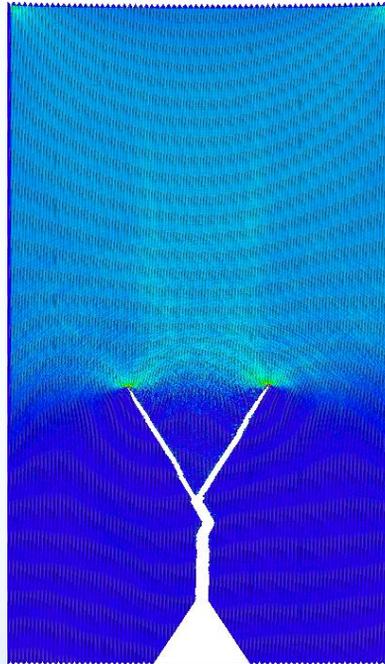
# LAMMPS CAC

## Verification: Crack Propagation

16,420  
Elements  
and 790k  
atoms



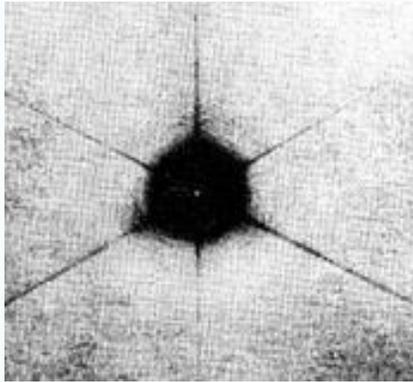
9.2 million  
atoms



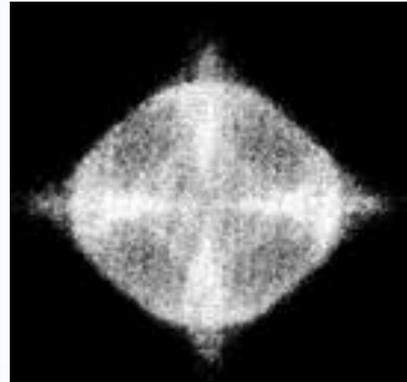
280 by 540 by 20 nm model loaded in tension along the x axis using an element volume of 400 unit cells. The crack is seen to branch in both the CAC and MD models with similar wavelike stress propagating from the crack tips.

# LAMMPS CAC

## Phonon Focusing Directions in Si



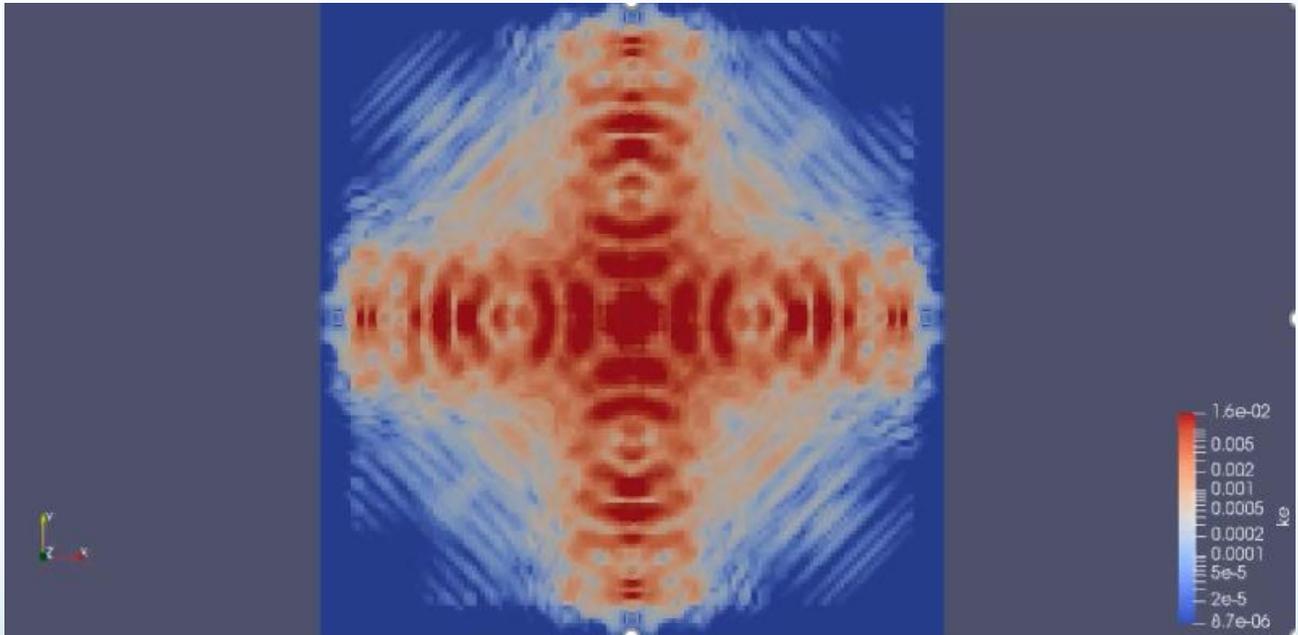
Six-fold Phonon Focusing seen on the <110> plane in Silicon. The image can be found in:  
Hauser, M. R., Weaver, R. & Wolfe, J. Internal diffraction of ultrasound in crystals: Phonon focusing at long wavelengths. *Physical review letters* **68**, 2604 (1992).



Four-fold Phonon Focusing seen on the <100> plane in Silicon. The image can be found in:  
Kolomenskii, A. A. & Maznev, A. A. Phonon-focusing effect with laser-generated ultrasonic surface waves. *Physical Review B* **48**, 14502-14508 (1993).

# LAMMPS CAC

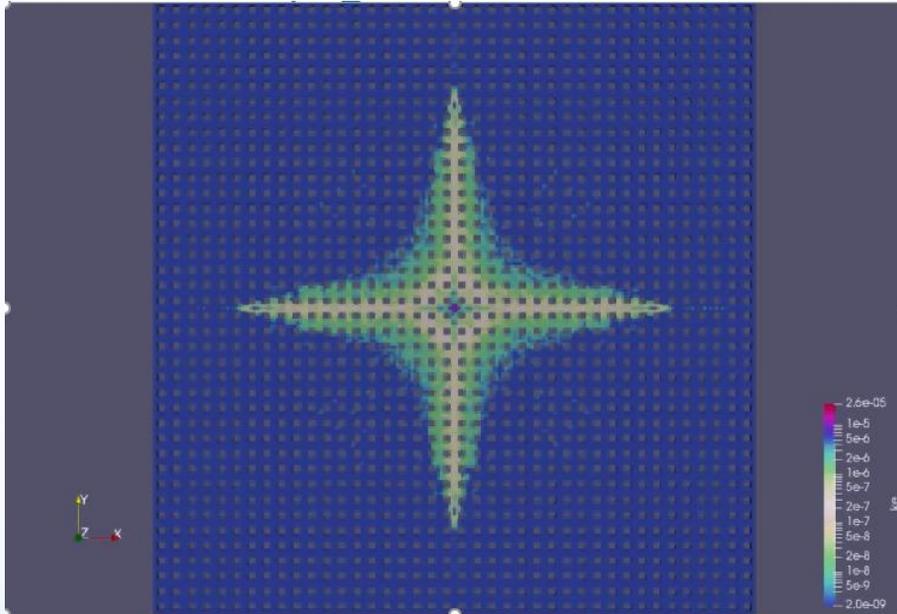
## Phonon Focusing Directions using SW silicon



800 nm by 800 nm by 5 nm plate model using cubic elements with a side length  $a = 54$  nm. The four-fold symmetry of kinetic energy can be seen by dividing the motif into four sections that are nearly identical.

# LAMMPS CAC

## Phonon Propagation and Microstructure



1400 nm by 1400 nm by 10nm plate model using cubic elements of side length  $a=85$  nm. The four-fold symmetry of kinetic energy can be seen even with the energy flow impeded along directions with many interfaces.

# LAMMPS CAC

## Summary

- The Completion of the CAC Algorithm on LAMMPS will enable a new range of simulations at the mesoscale involving the dynamic coupling of microstructure, defects, and waves.
- Such simulations can be performed at length scales previously unexplored with a formalism that needs no additional rules or parameters other than the interatomic interaction, similar to MD.
- LAMMPS will probably include the CAC method by the time of the Fall stable release unless major issues are discovered; No promises 😊.