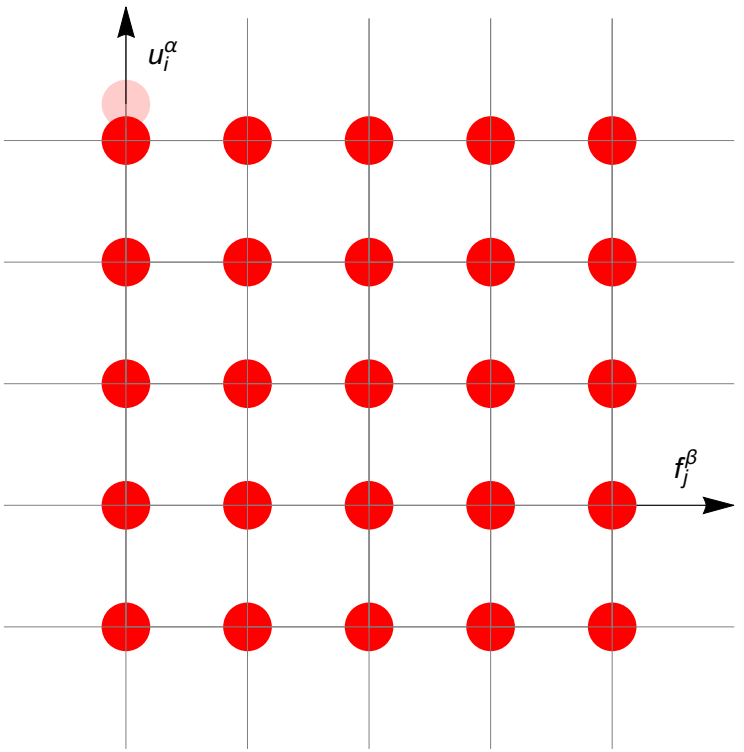
Phonon spectra from the supercell method

19 January 2017

The supercell method

- displace ion i in direction α by small distance $\pm u_i^\alpha$
- evaluate forces on every ion in the system due to displacement ($f_{j,\beta}^+$ and $f_{j,\beta}^-$)
- compute the derivative numerically using the central difference form and obtain real space force constant matrix



$$\Phi_{ij}^{\alpha\beta} = \frac{\partial^2 E}{\partial u_i^\alpha \partial u_j^\beta} = \frac{f_{j,\beta}^- - f_{j,\beta}^+}{2u_i^\alpha}$$

The supercell method

- relies on linearity of the forces (small displacements)
- relies on short-range nature of interatomic force constant matrix

  $\Phi_{ij}^{\alpha\beta}(R) \to 0$ as $R \to 0$
- requires in general $3n_{at}$ displacements, with n_{at} being the number of atoms in the primitive cell
- reconstruct force constant matrix by making use of symmetry to avoid computing symmetry equivalent perturbations

The supercell method

- compute fourier transform and obtain $D_{st}^{\alpha\beta}(\mathbf{q})$

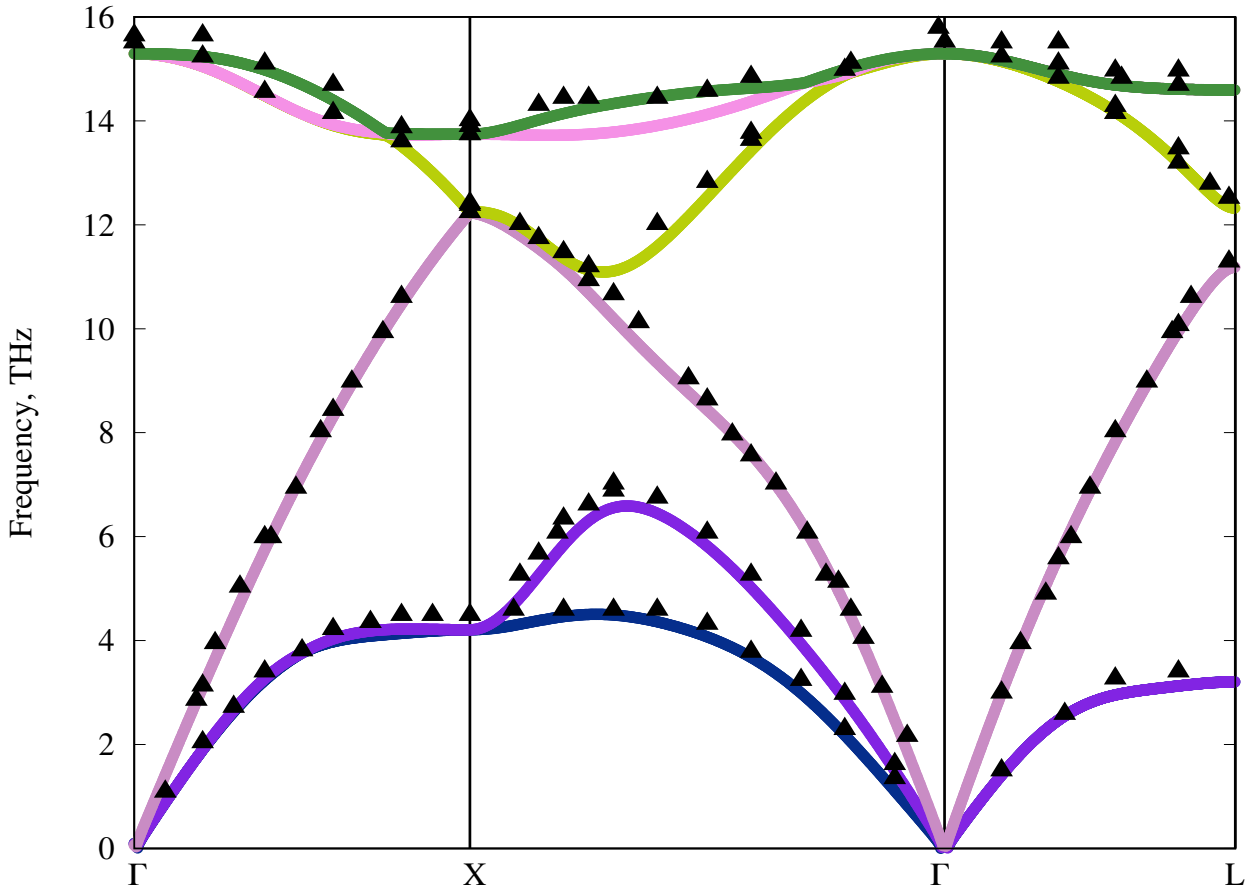
$$D_{st}^{\alpha\beta}(\mathbf{q}) = \sum_{l=0}^{N_{cell}-1} \Phi_{0s,lt}^{\alpha\beta} e^{i\mathbf{q}(\mathbf{R_l}-\mathbf{R_0})}$$

- diagonalize $D_{st}^{\alpha\beta}(\mathbf{q})$ to obtain eigenvalues and eigenvectors

The supercell method: how to run

- **python3 script_1.py** - compute interatomic force constant matrix
- script_1.py should produce **ifcfile_fd**
- **python3 script_2.py** - to compute and plot the spectra
- **evince spectra_fd.pdf** - to visualize the plot

Phonon spectra for fcc Si



▲ - experimental data

G.Nilsson and G.Nelin, Phys. Rev. B 6, 3777 (1972)

J. Kulda, D. Strauch, P. Pavone, and Y. Ishii, Phys. Rev. B 50, 13347 (1994)