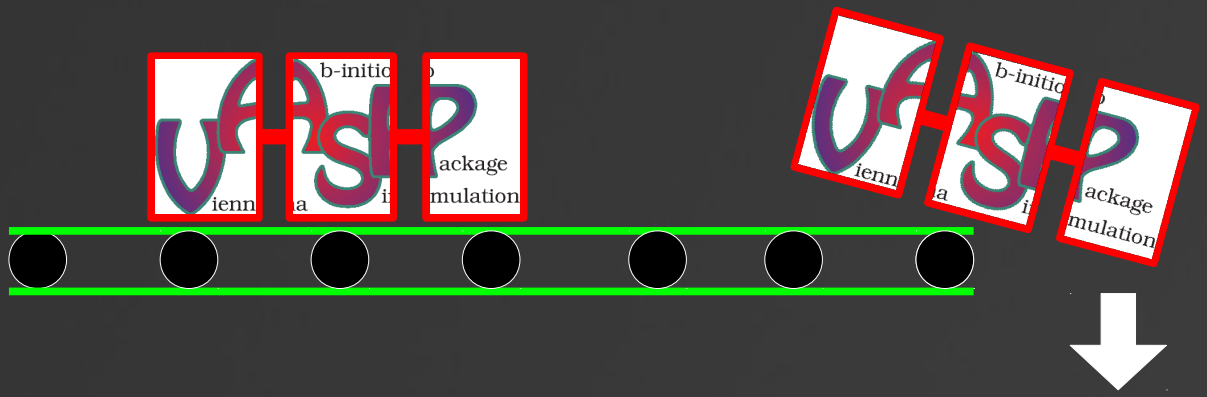
# Automation system
# Cogue

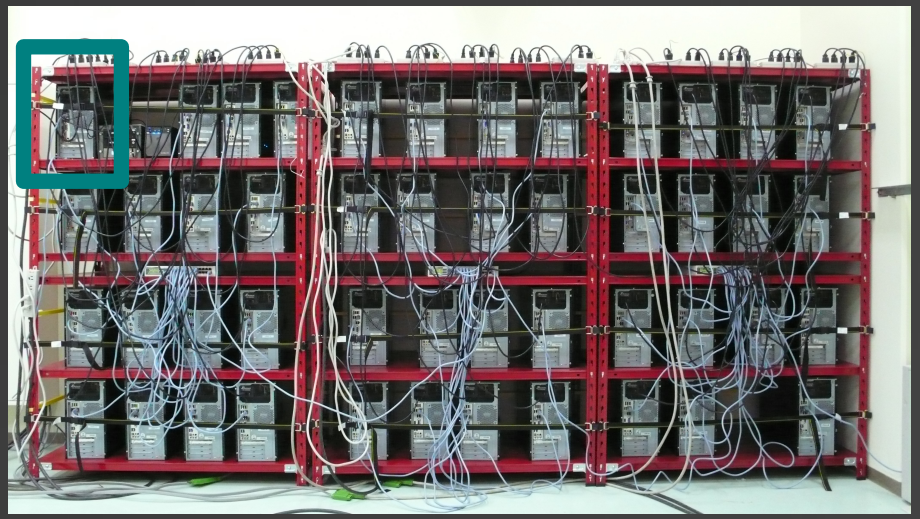
https://github.com/atztogo/cogue

Atsushi Togo*[1] and Isao Tanaka[1,2]

[1]Elements Strategy Initiative for Structural Materials, Kyoto University
[2]Department of Materials Science and Engineering, Kyoto University

# Automation with queueing system

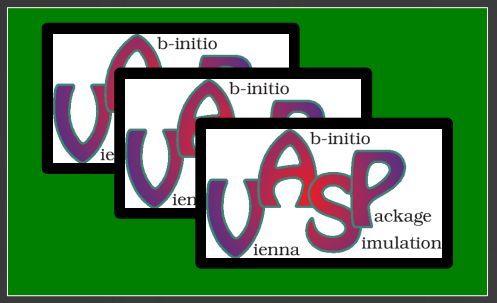




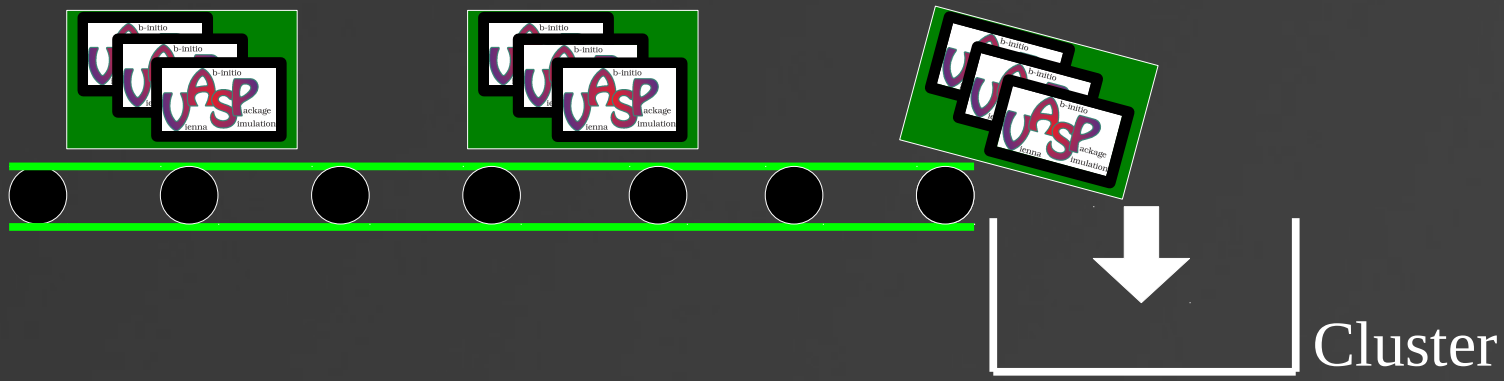
# Automation

- Automation is hierarchical.
  - VASP calculation, well automated.


  - Bunch of VASP calculations may be automated by a shell-script.

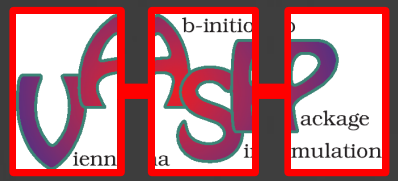



  - Shell-scripts may be automatically and flexibly executed on a computer cluster using a queueing system.

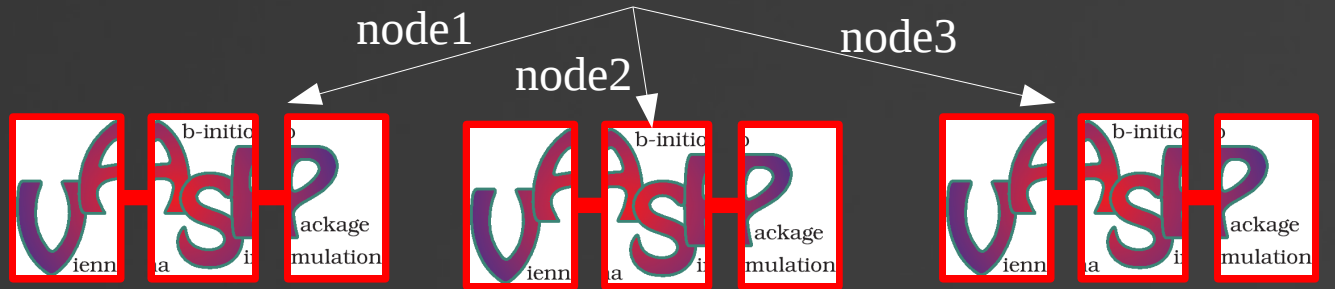


# Distributed computation

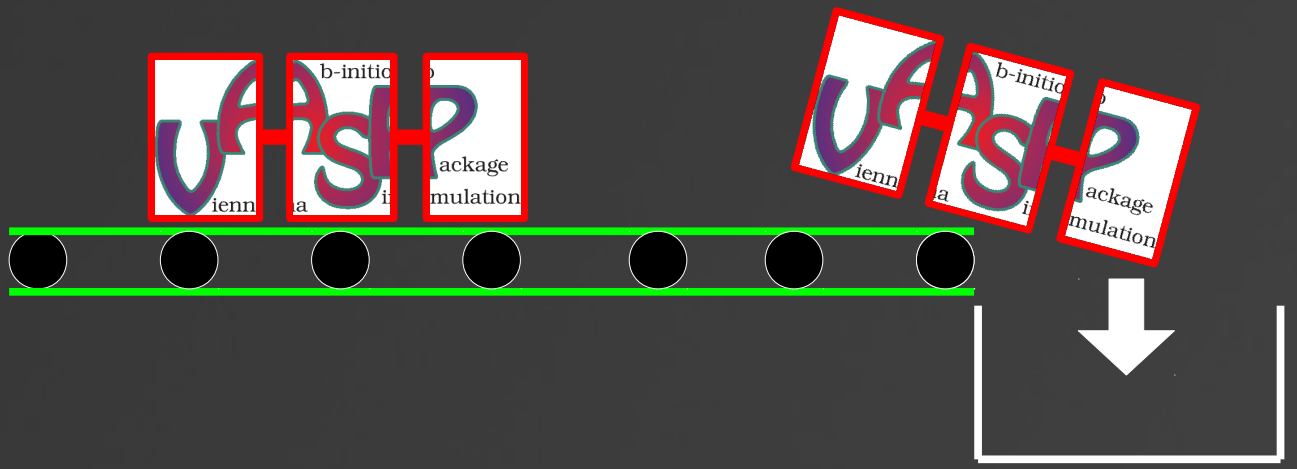
- Distribution is hierarchical.
  - VASP calculation, well distributed by MPI



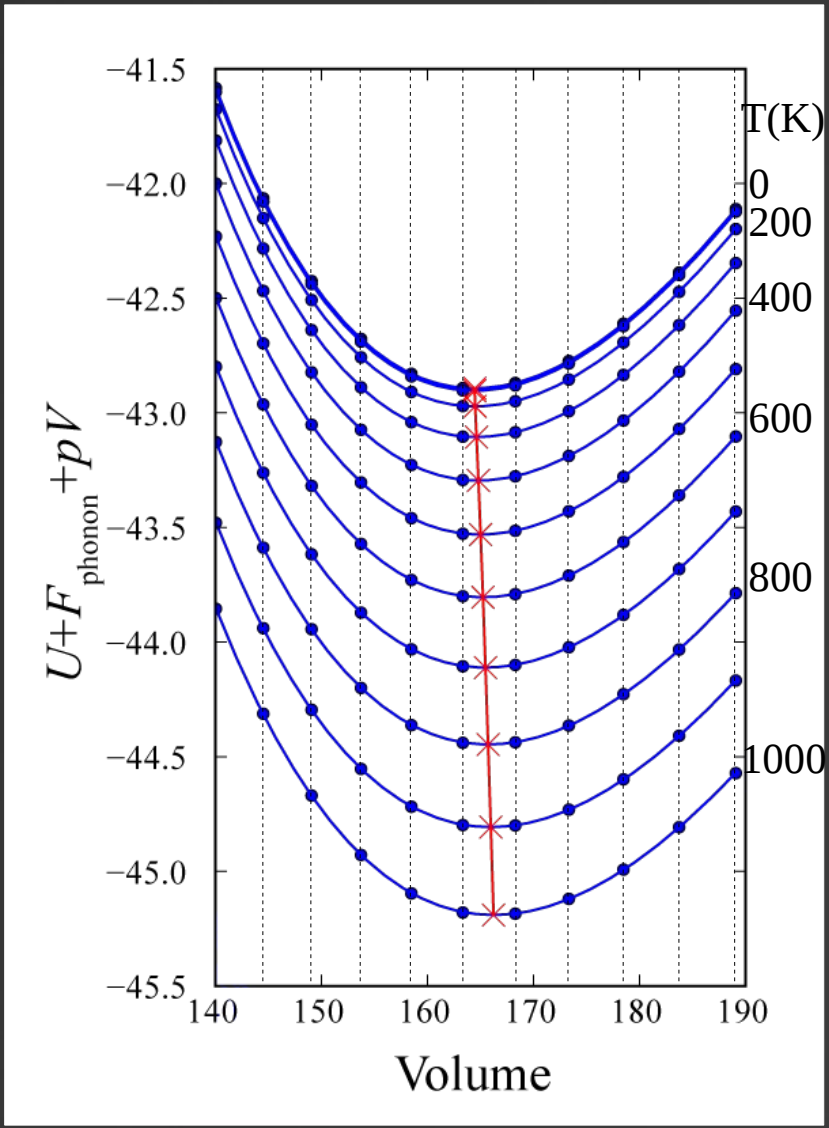
  - Maybe distributed by a shell-script.




  - Maybe distributed using a queueing system.

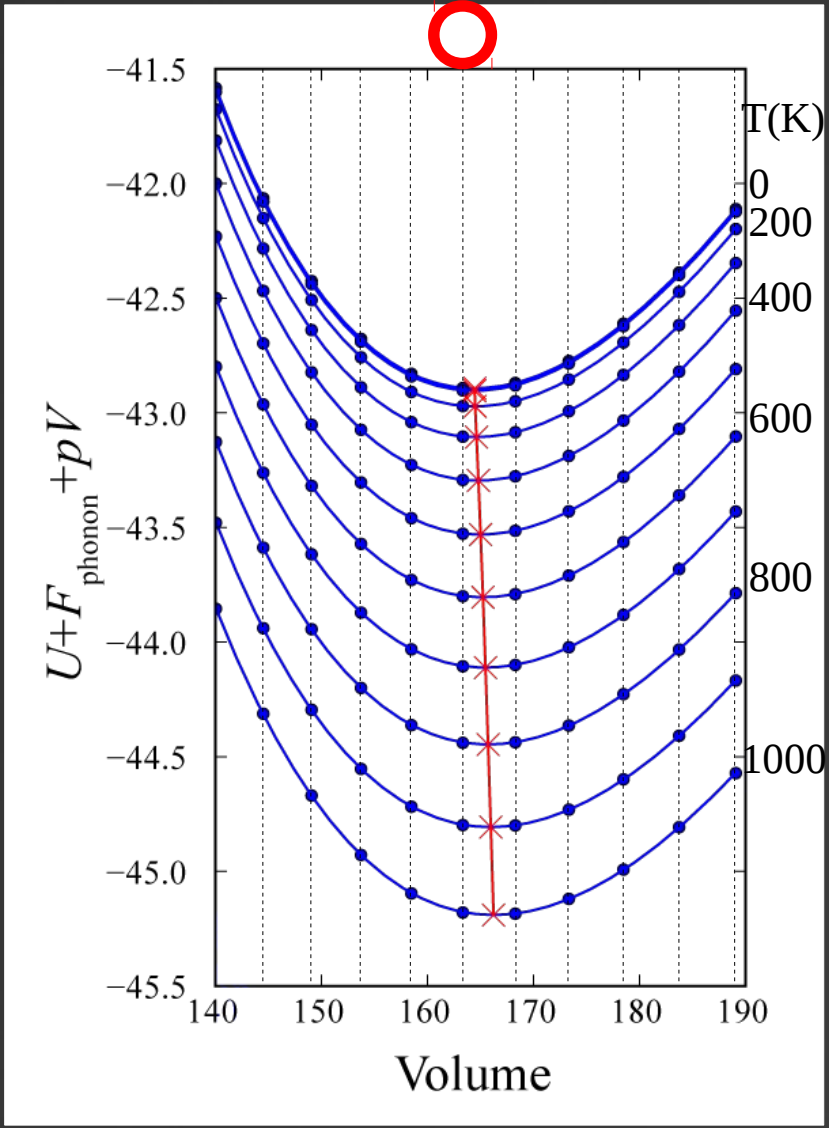


# Example:
# Thermal expansion calculation




1. Structure optimization of a unit cell
2. Create 10 unit cells with different volumes
3. Structure optimization of 10 unit cells
4. 11 phonon calculations
5. Quasi-harmonic fitting

# Diagram of thermal expansion calculation

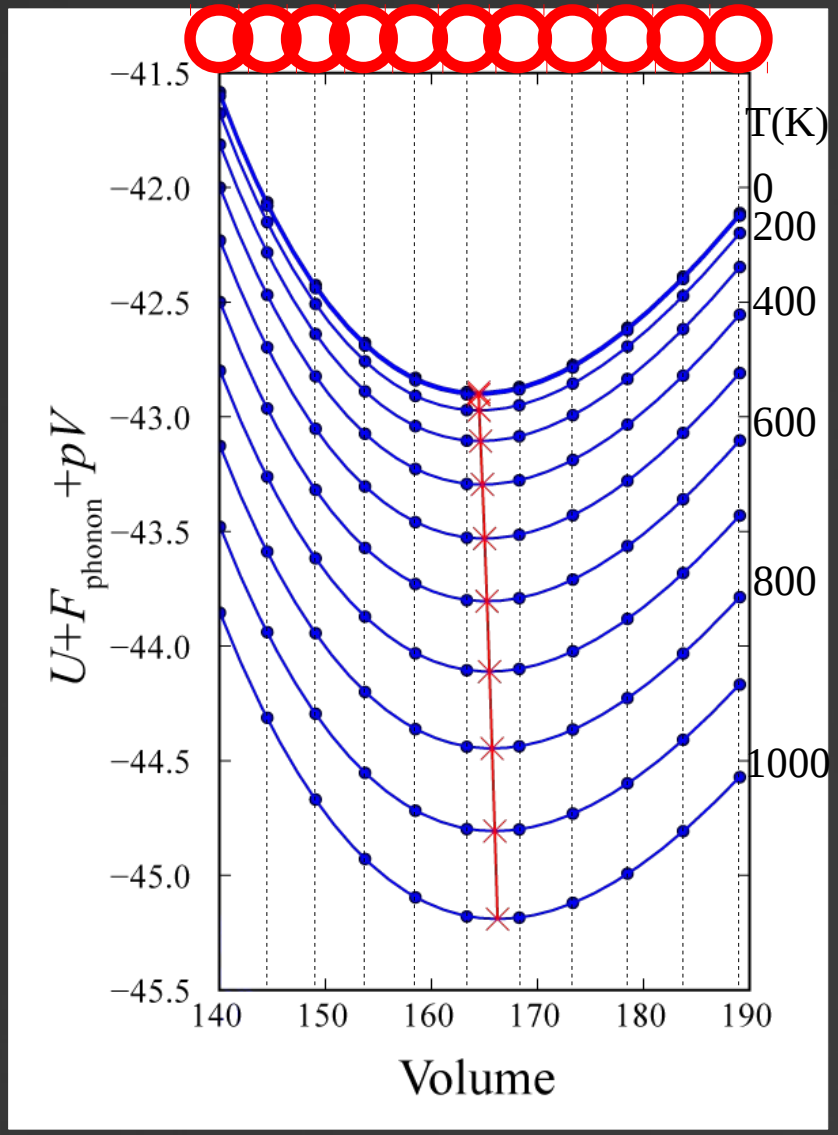



Structure optimization

Stage 1

Determine initial volume

# Diagram of thermal expansion calculation



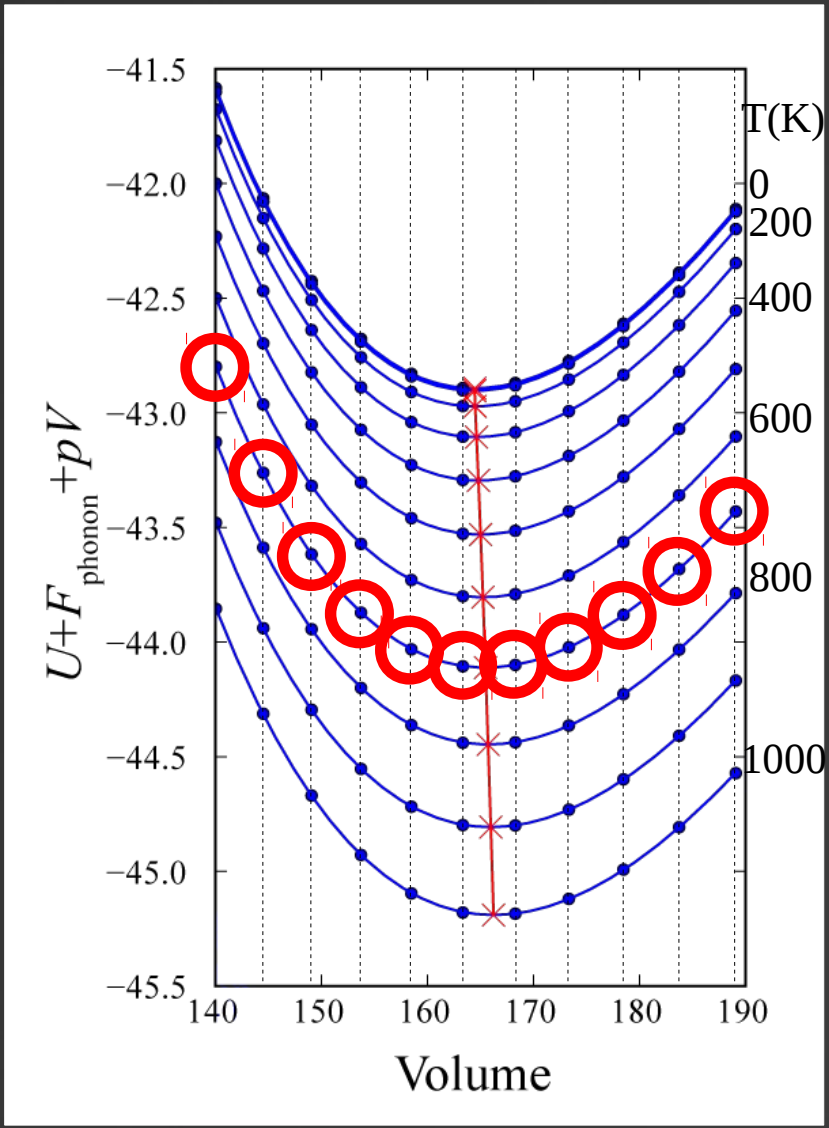

Structure optimization

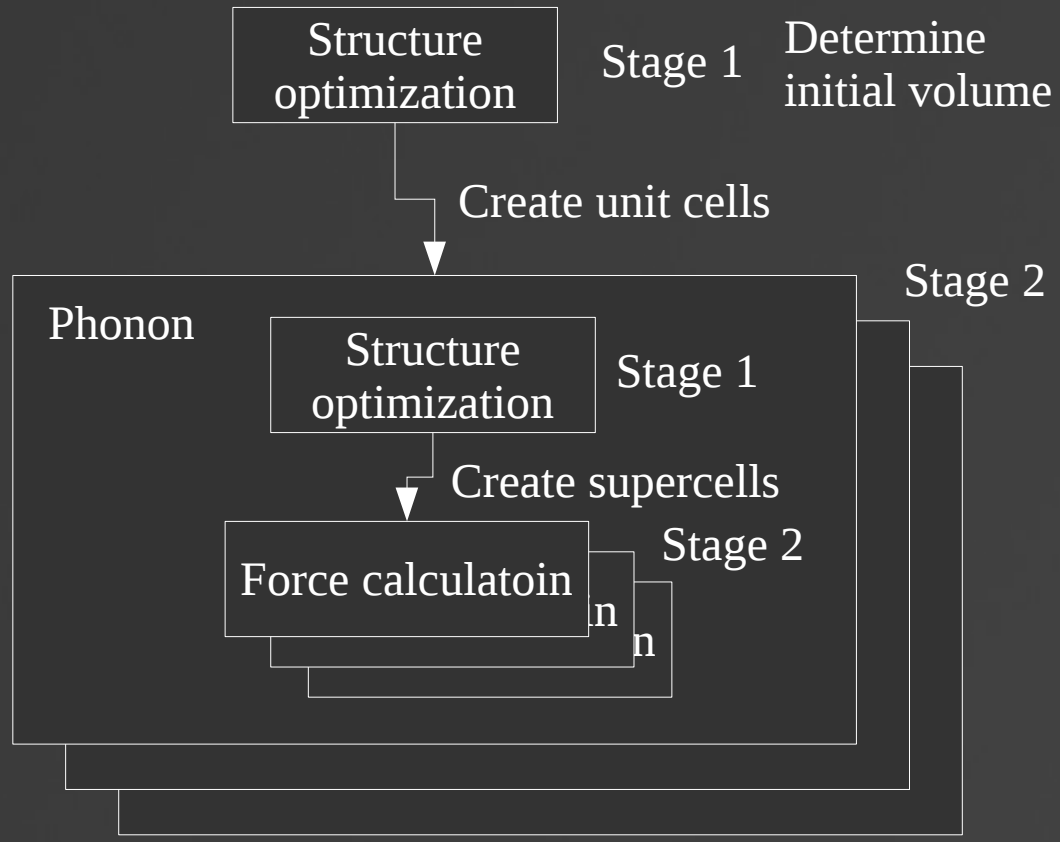
Stage 1

Determine initial volume

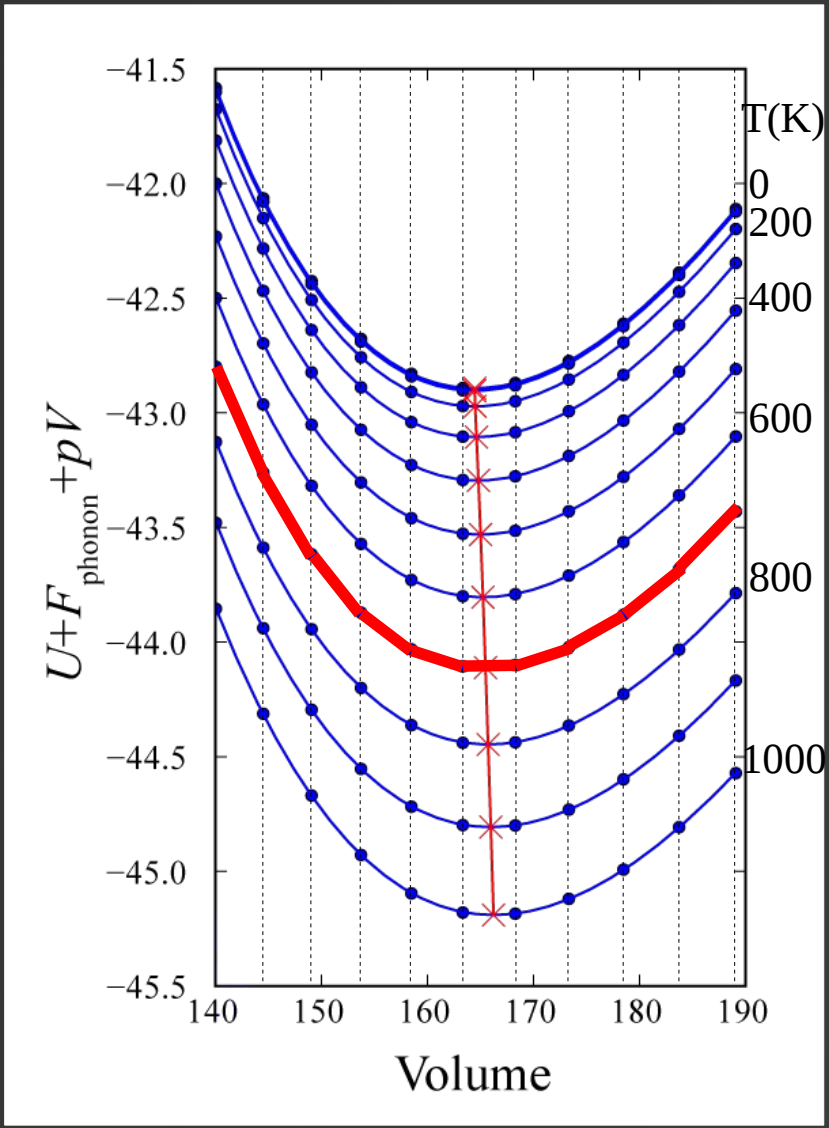
Create unit cells

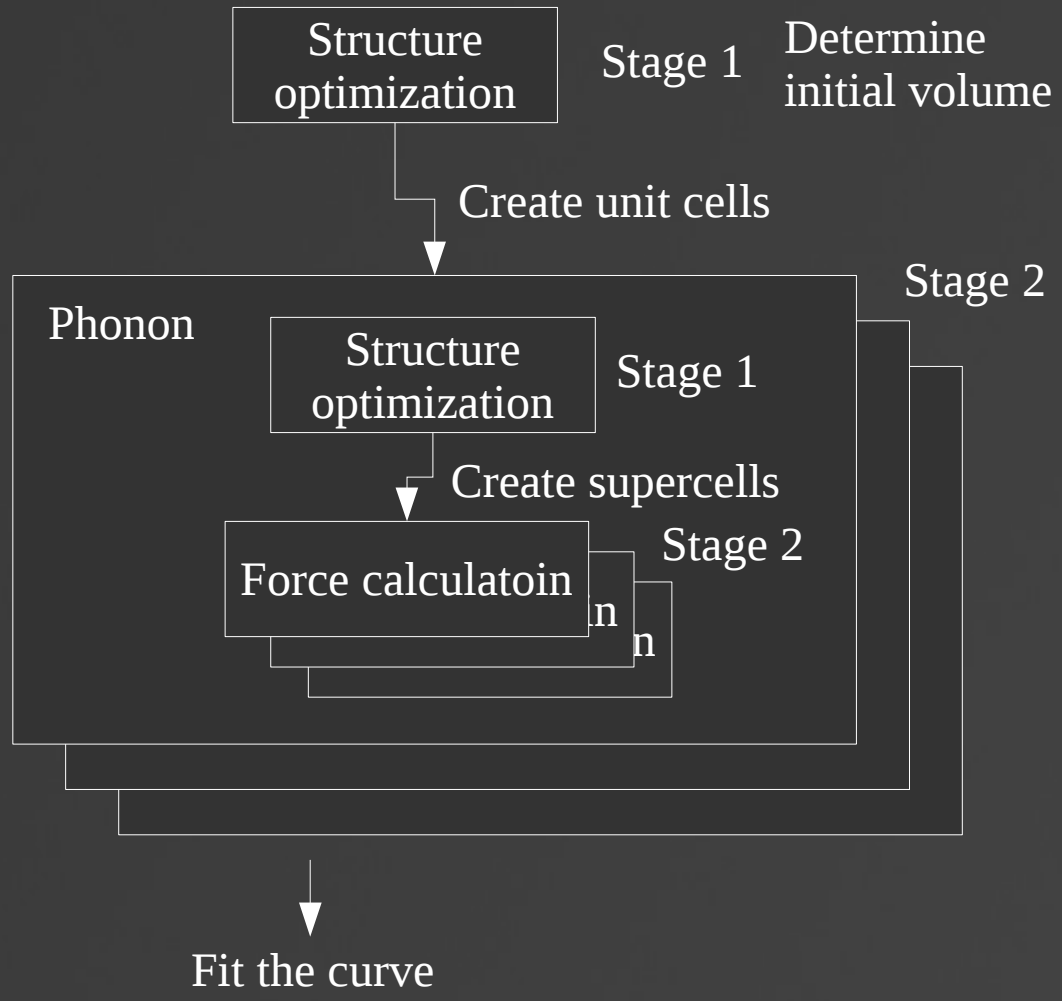
# Diagram of thermal expansion calculation



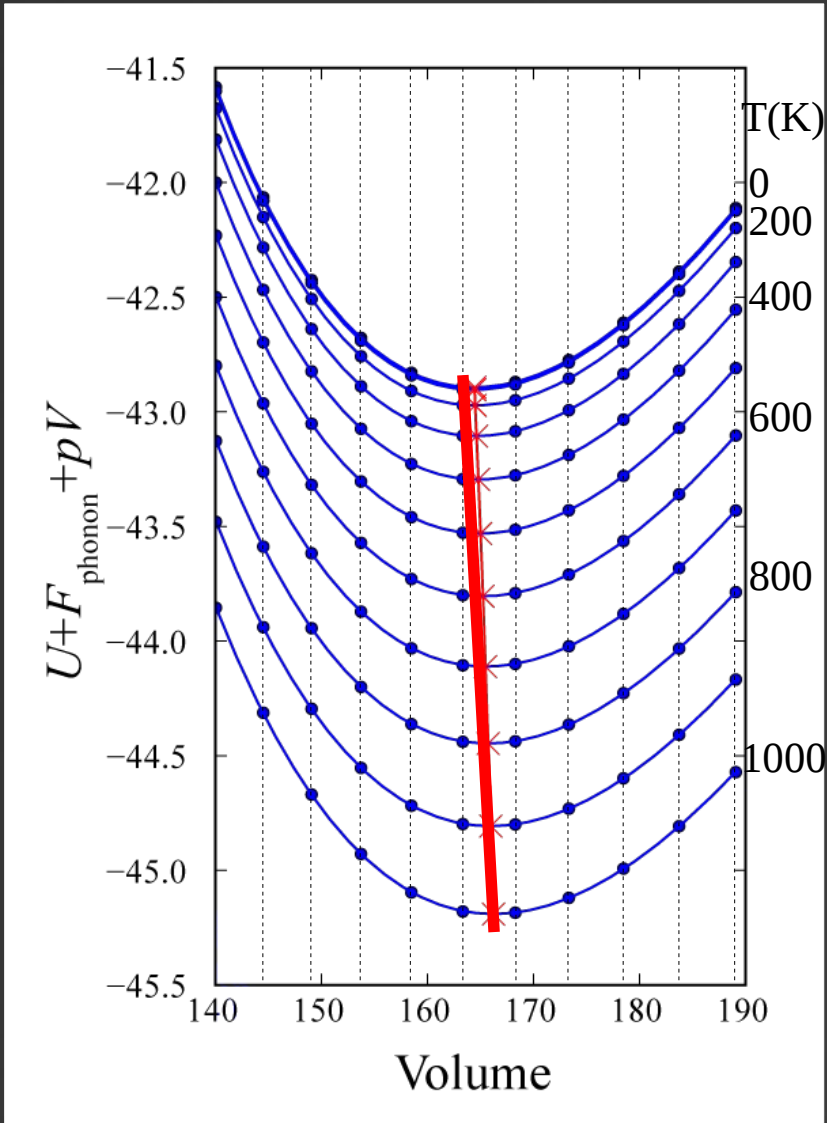



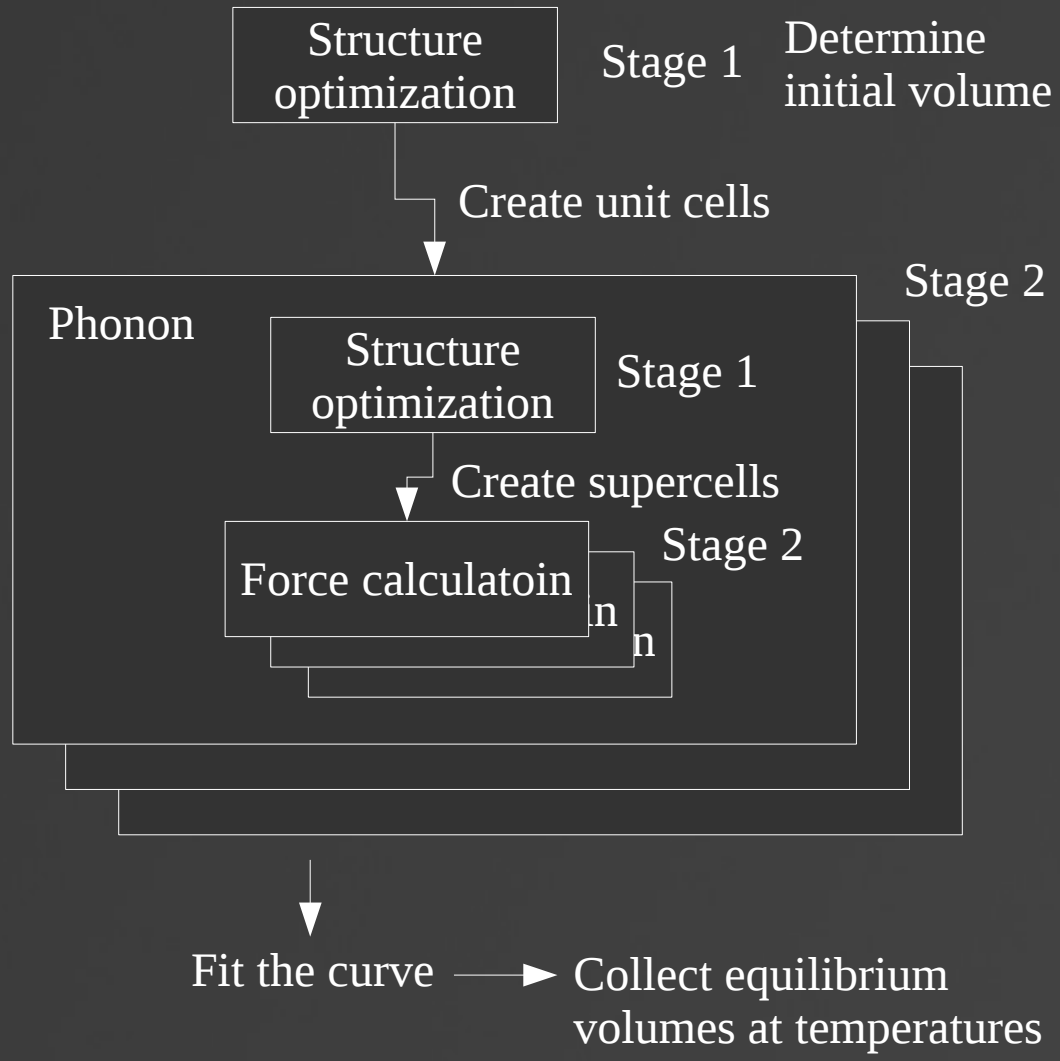
# Diagram of thermal expansion calculation



# Diagram of thermal expansion calculation

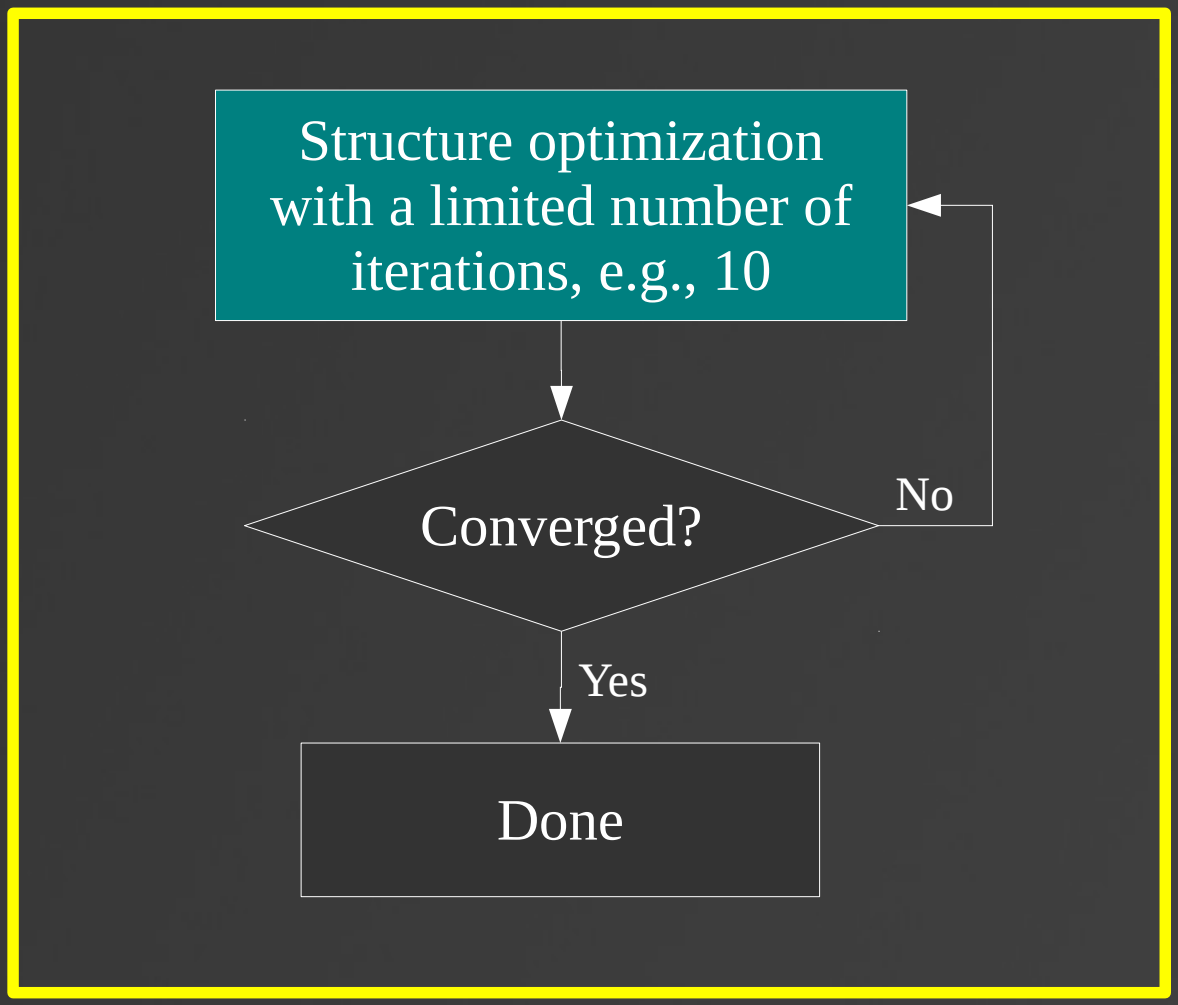


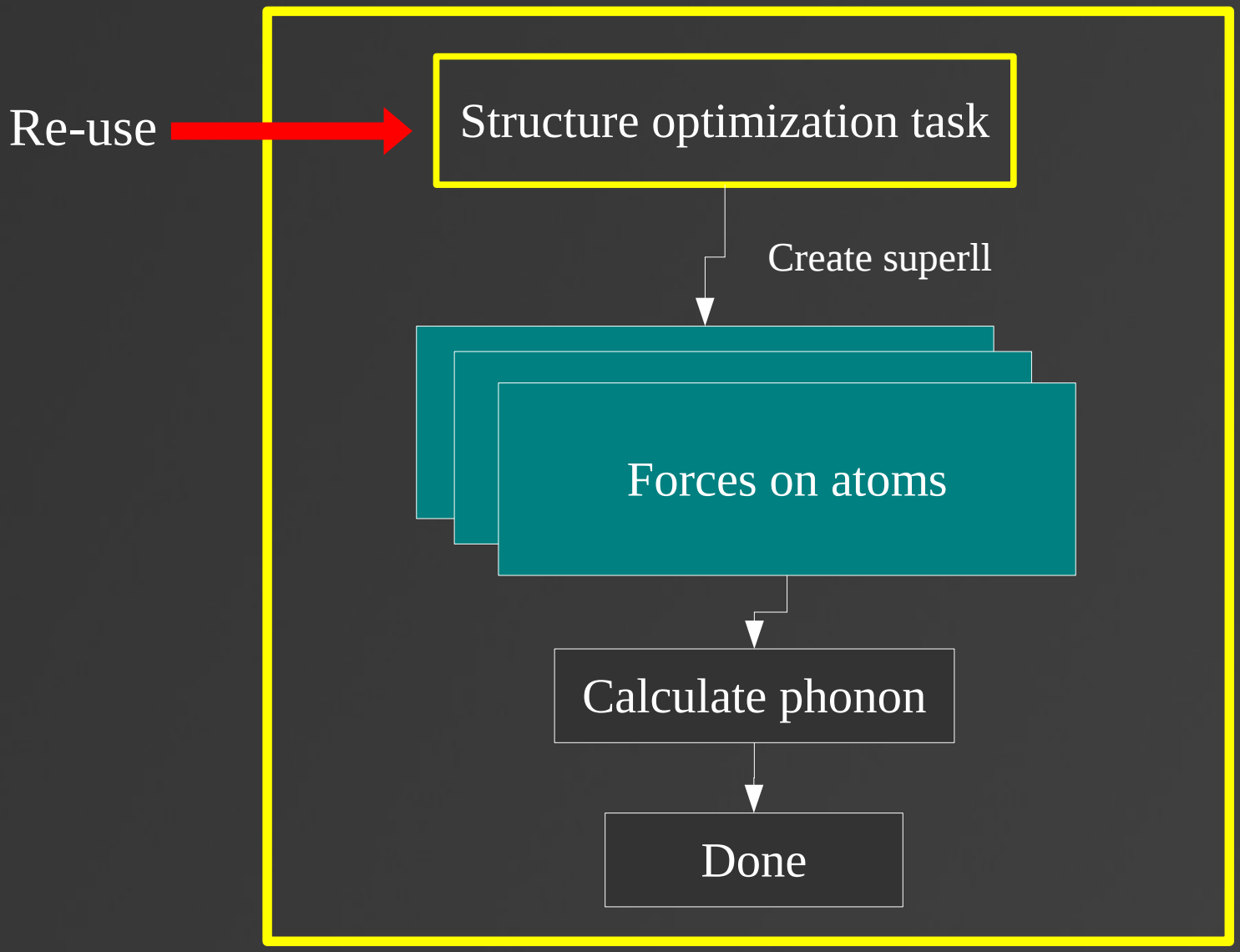
# Implementations of execution tasks that are submitted to queueing system

| | |
|---|---|
| Structure optimization with a limited number of iteration, e.g., 10 | Forces on atoms |
| Energy | Stress |
| Elastic constants | Dielectric constant<br>Born effective charges |

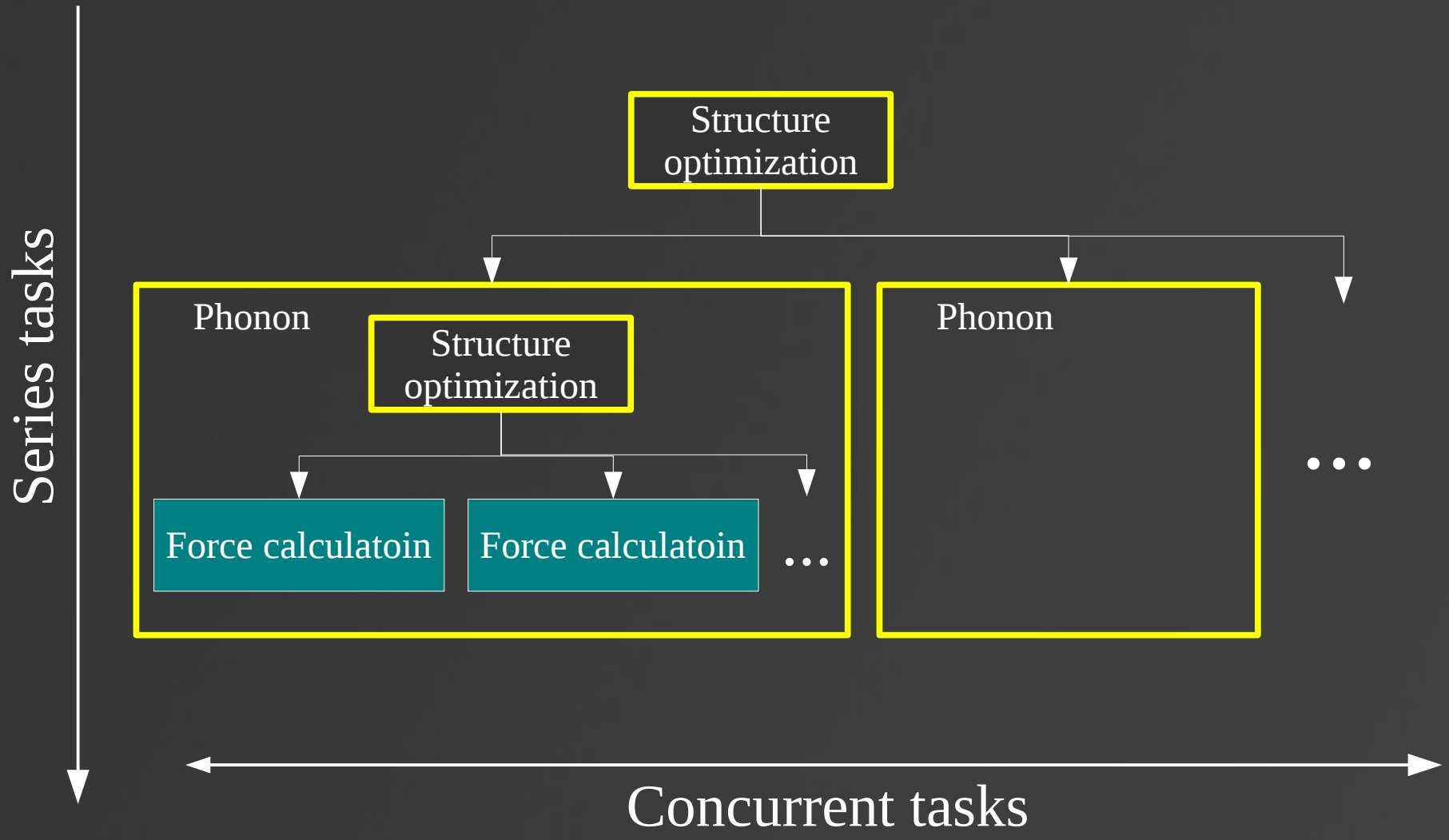
# Implementation of general structure optimization task



# Implementation of phonon task



# Implementation of thermal expansion calculation



# Kernel of automation system

```
def _deep_run(self, task):
    cwd = self._chdir_in(task.get_directory())

    subtasks = task.get_tasks()
    if subtasks: # taskset
        for subtask in subtasks:
            if not subtask.done():
                self._deep_run(subtask)

    else: # job task
        self._queue.set_job_status(task)

    task.set_status()
    if task.done():
        try:
            next_subtasks = task.next()
        except StopIteration:
            task.end()
        else:
            for next_subtask in next_subtasks:
                self._deep_begin(next_subtask)

    self._chdir_out(cwd, task.get_status())
```

Concurrent tasks

Recursive call of subtask

Series task

*Standardization

To control tasks, each task has to hold the following methods:

| | |
|---|---|
| Task.begin() | Task.end() |
| Task.next() | Task.done() |

# Script for bulk modulus calculation

```python
#!/usr/bin/env python

import numpy as np
import cogue
import cogue.calculator.vasp as vasp
import cogue.qsystem.gridengine as ge

task_name = "sno2"

# Crystal structure
symbols = ['Sn'] * 2 + ['O'] * 4
lattice = [[4.75, 0, 0],
           [0, 4.75, 0],
           [0, 0, 3.25]]
points=np.transpose([[0.0, 0.0, 0.0],
                     [0.5, 0.5, 0.5],
                     [0.3, 0.3, 0.0],
                     [0.7, 0.7, 0.0],
                     [0.2, 0.8, 0.5],
                     [0.8, 0.2, 0.5]])
cell = cogue.cell(lattice=lattice,
                  points=points,
                  symbols=symbols)

# Vasp settings
ps_map = {'Sn': 'Sn_PBE',
          'O': 'O_PBE'}
incar = vasp.incar()
incar.set_structure_optimization()
incar.set_encut(400)
incar.set_prec("Normal")
```

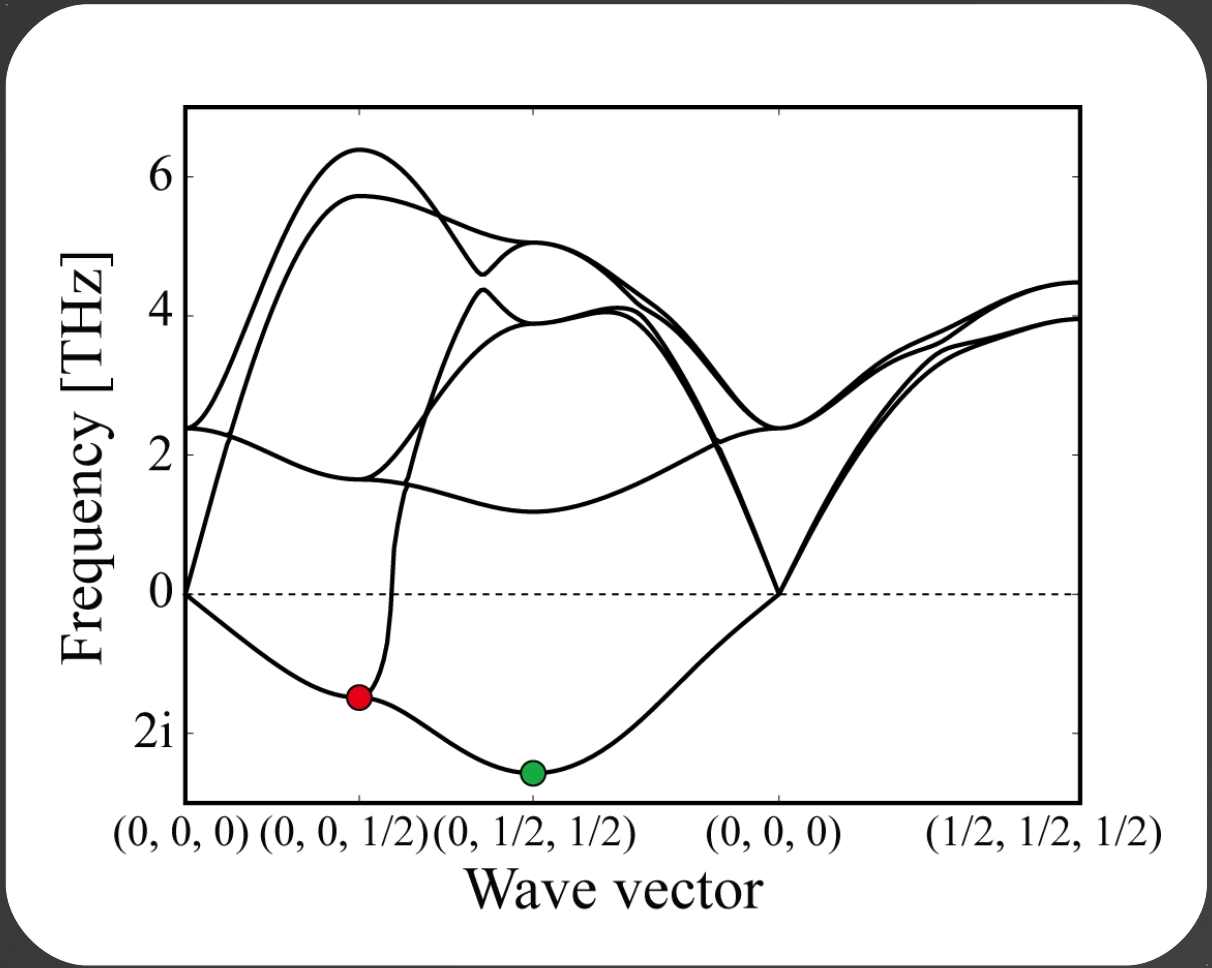
```python
# Queue
job = ge.job(script="vasp5212serial",
             shell="/bin/zsh",
             jobname=task_name,
             stdout="std.log",
             stderr="err.log")

# Task
task = vasp.bulk_modulus(max_iteration=2,
                         cell=cell,
                         pseudo_potential_map=ps_map,
                         k_mesh=[4, 4, 6],
                         incar=incar,
                         job=job)

# Automatic calculation
calc = cogue.autocalc()
calc.append(task_name, task) # More tasks can be appended.
calc.set_queue(ge.queue())
calc.run(check_period=5)
print "space group:", cogue.symmetry(cell)['international']
print "status:", task.get_status()
# 201.411956183 GPa
print "bulk modulus:", task.get_bulk_modulus(), "GPa"
```

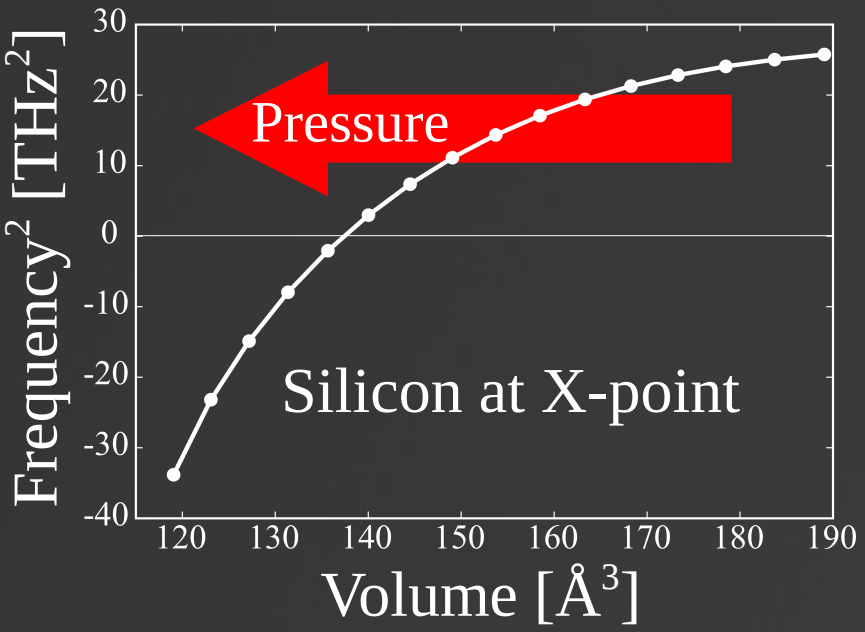
# Application of metastable structure search

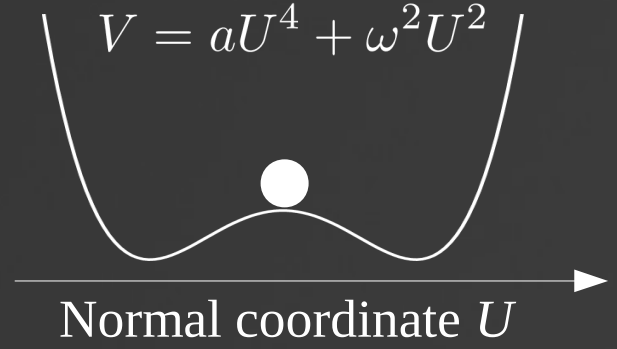
A hypothetical structure: CsCl-type NaCl at $p$=0

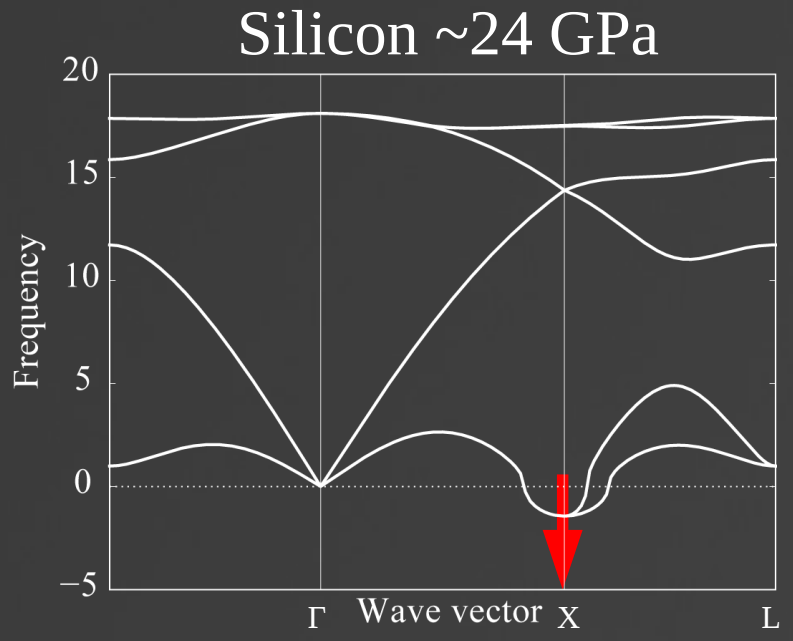


# $\omega^2 < 0$: Instability of crystal potential

$$\mathrm{D}(\mathbf{q})\mathbf{e}(\mathbf{q}s) = [\omega(\mathbf{q}s)]^2\mathbf{e}(\mathbf{q}s)$$



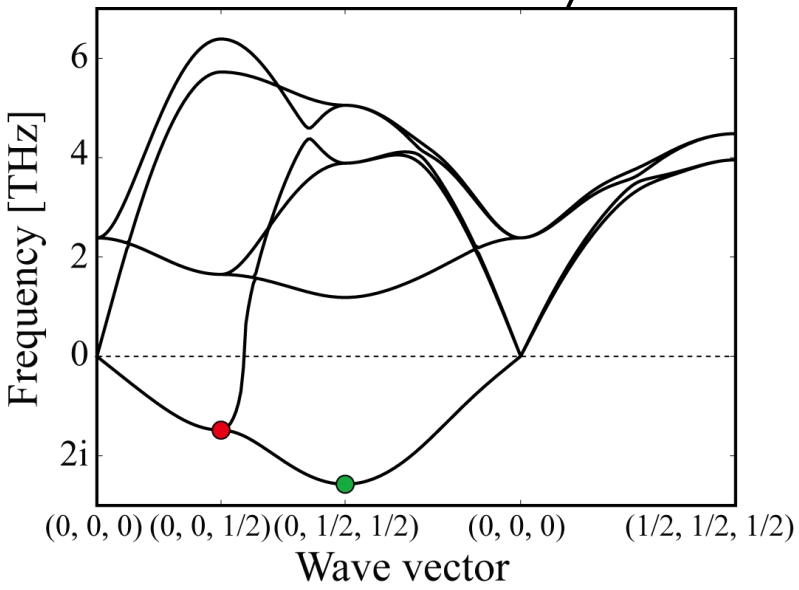



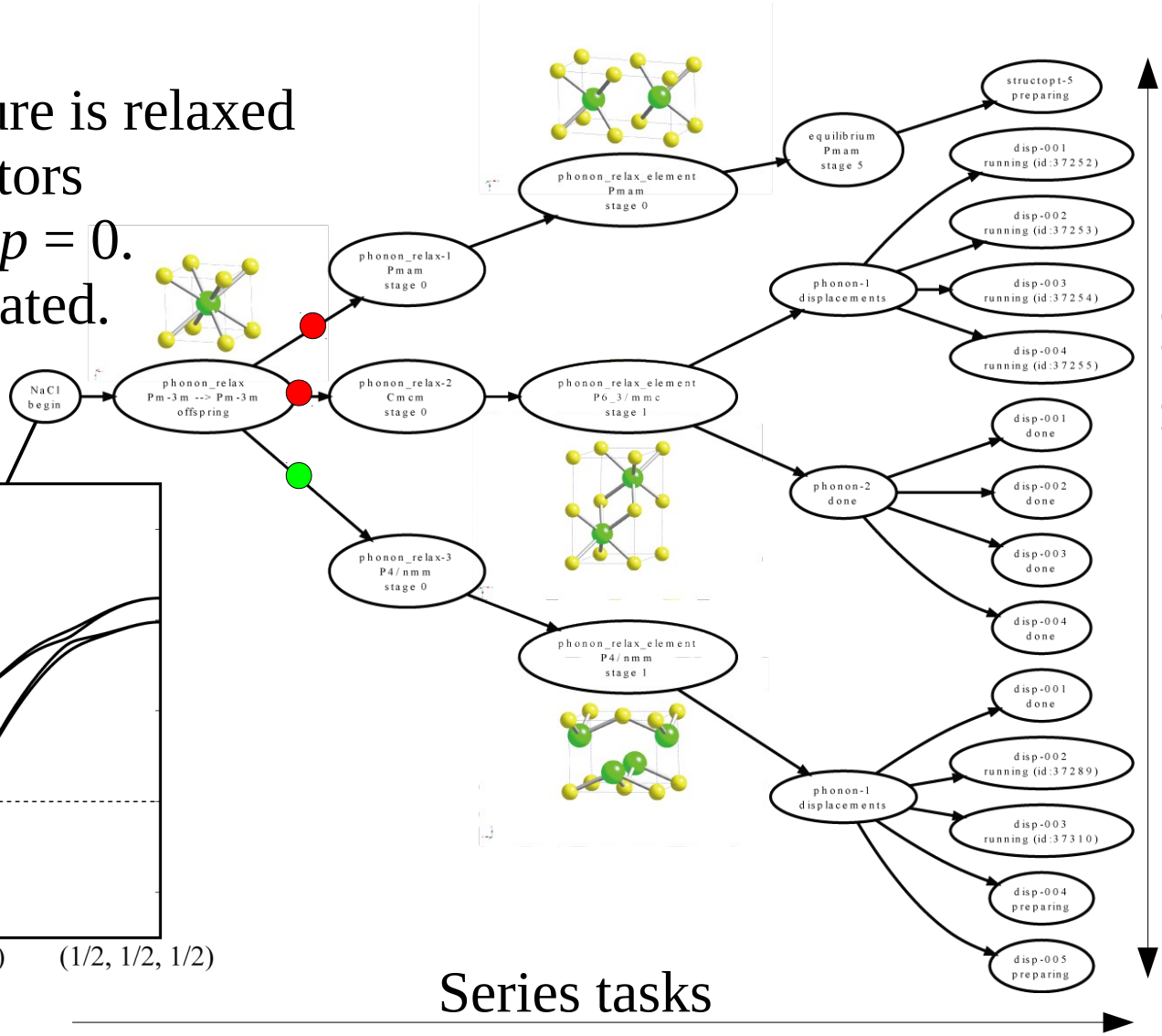




*Imaginary frequencies are shown by negative values.

# Automatic structure relaxation

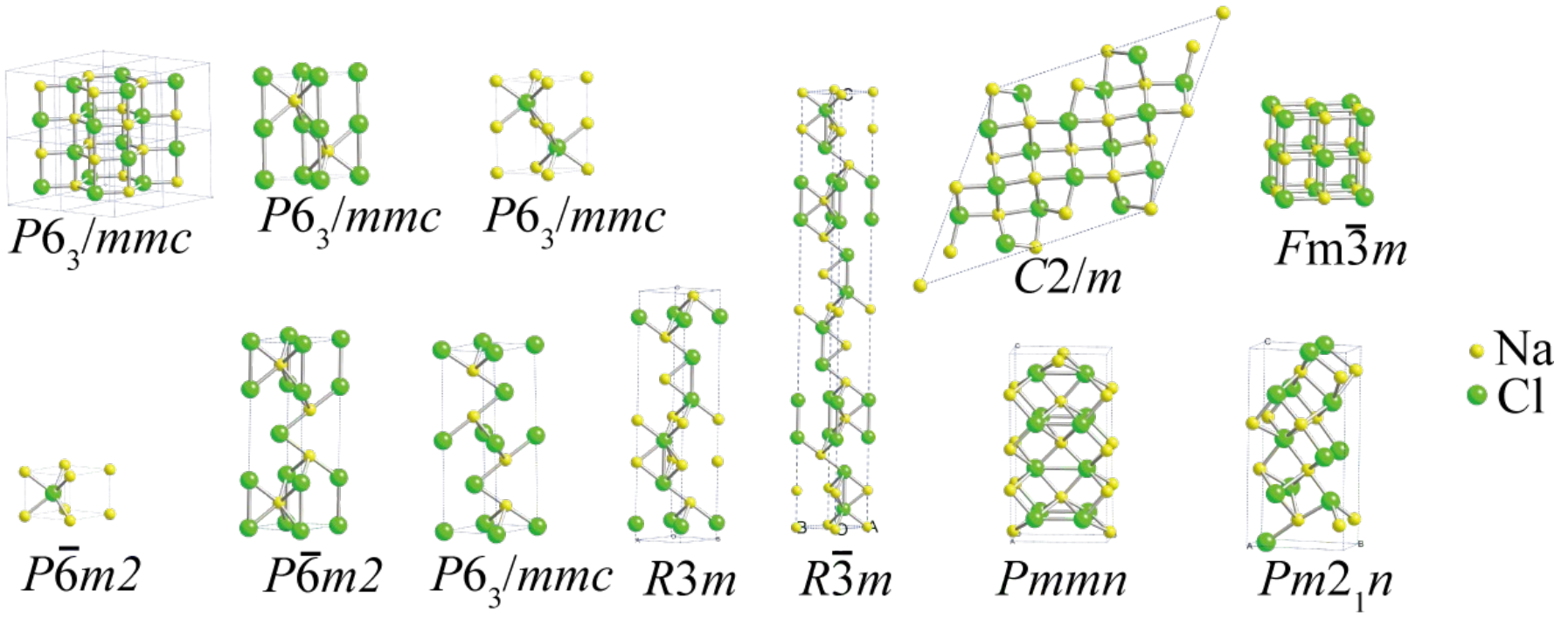
CsCl-type NaCl structure is relaxed following the eigenvectors of imaginary modes at $p = 0$. Calculations are automated.




*Number of series tasks increases on-the-fly.

# Dynamically stable structures of NaCl




Most of the structures were found as close-packed alternate stacking of Na and Cl layers.

*See for more details, Togo and Tanaka, Phys. Rev. B 87, 184104 (2013)