Scriptable Calculation Environment for Crystal Simulations Working with Queueing System

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For the research that requires complicated handling of a bunch of computing steps, we have been developing a scriptable calculation environment [1]. One of the aims of this development is to provide recipes of automations of crystal simulations. As an example, a workflow of a phonon calculation with the supercell method is shown in Fig. 1. After initializing the phonon calculation (Begin), an input unit cell structure is optimized until the residual forces on atoms become less than some small enough values under some lattice or stress constraint (Stage 1). The supercells with atomic displacements are created from the optimized unit cell (Next). Then a bunch of force calculations are executed (Stage 2). Finally the phonon properties are calculated from the calculated forces on atoms of supercells (End). In this example, the first-principles calculations are executed in the stages 1 and 2. The jobs are submitted to a computing cluster by using a queueing system. The statuses of the jobs are monitored. After all the jobs at each stage finish, the phonon calculation proceeds to the next step. In the stage 2, the force calculations are automatically distributed and the first-principles calculations are executed concurrently.

A pattern of tasks is employed in the framework of the calculation environment. The 'Begin', 'Next', and 'End' shown in Fig. 1 are the functions that are always called by an outside controller, which is a part of the pattern. A task is composed of a series of tasks. By describing a task under the pattern, the controller needs not to know the details of tasks. Since the phonon calculation is also a task, this can be used for a more complicated task. In Fig. 2, the phonon calculations are used as tasks to calculate thermal expansion. The algorithm of the framework is simple. The series of simulation steps is implemented by an iterator [2]. The task nesting is achieved by a recursion [3]. An interesting feature of this calculation environment is that simulation steps can be generated on the fly. This is important for the structure optimization since it is initially unknown how many times of the iterations is required. Like the structure optimization, calculations of physical properties are considered as applications of this calculation environment.

The computer program of the calculation environment is coded mostly in Python language. Crystal symmetry tools with spglib [4] are bundled. The queueing system and the first-principles calculations are wrapped by the calculation environment. Currently the wrappers of Grid Engine [5] and VASP code [6] are prepared.

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References
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[3] http://en.wikipedia.org/wiki/Recursion_(computer_science)
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[5] http://gridengine.org/
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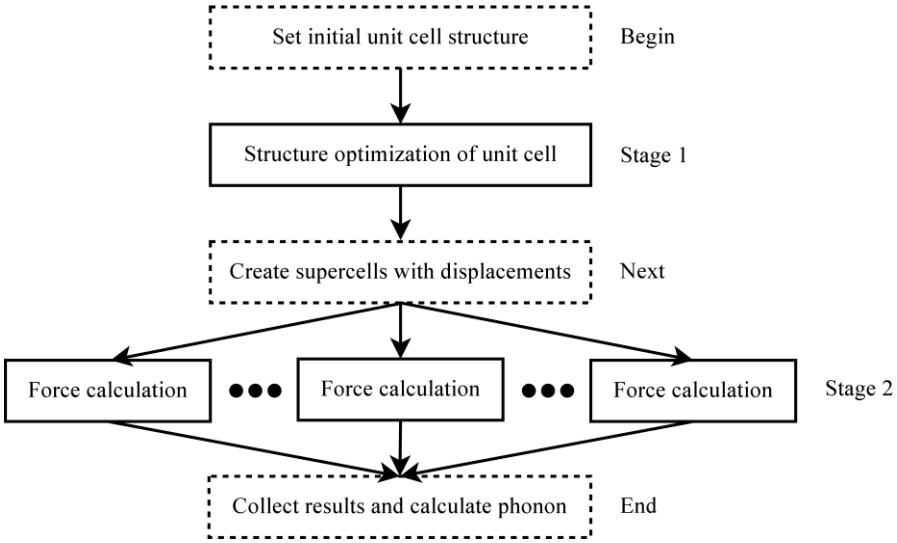

FIG. 1. Work flow of phonon calculation with the supercell method.

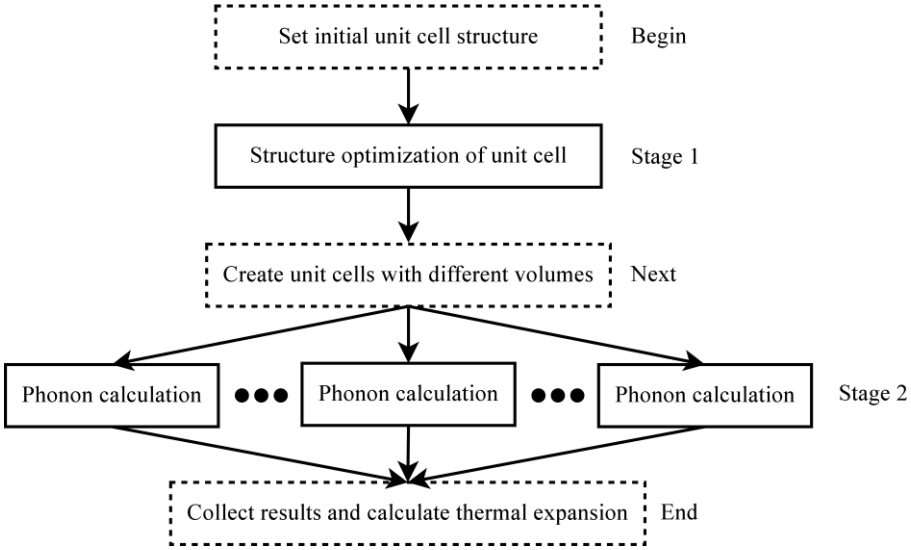

FIG. 2. Work flow of thermal-expansion calculation under the quasi-harmonic approximation.