591V Multiscale Materials Modeling

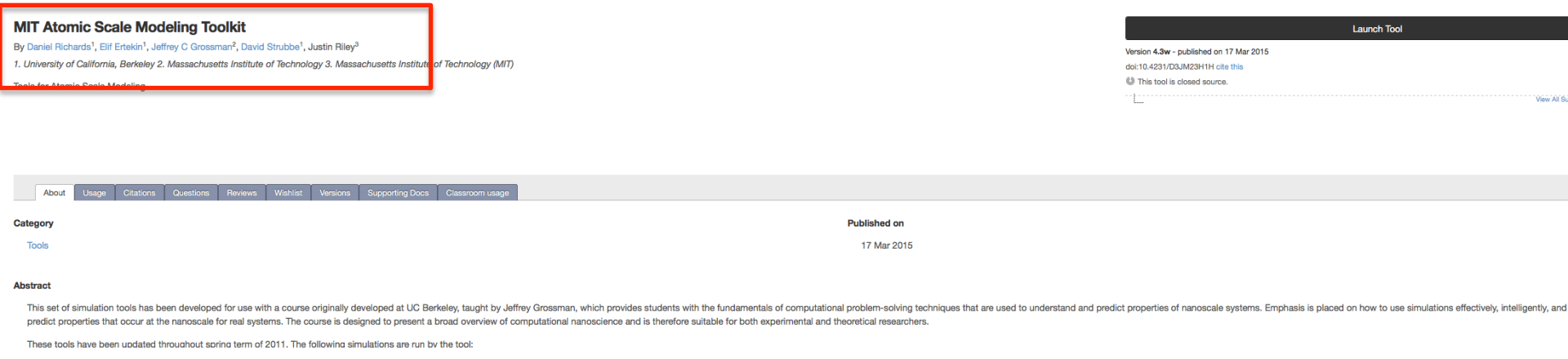
Computational Lab-3

Outline: Today's class

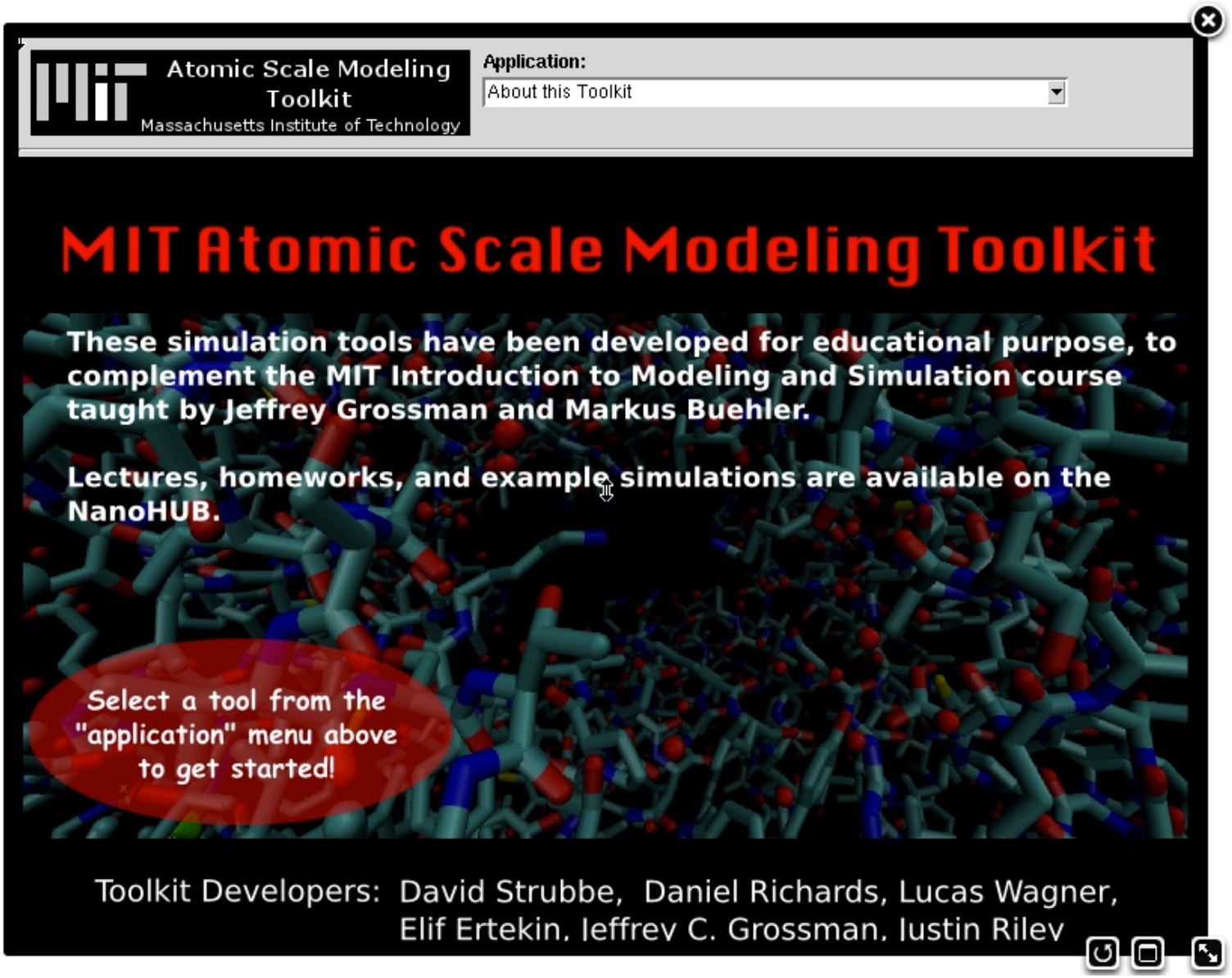
Outline:

Using atomic scale modeling kit (PWSCF)

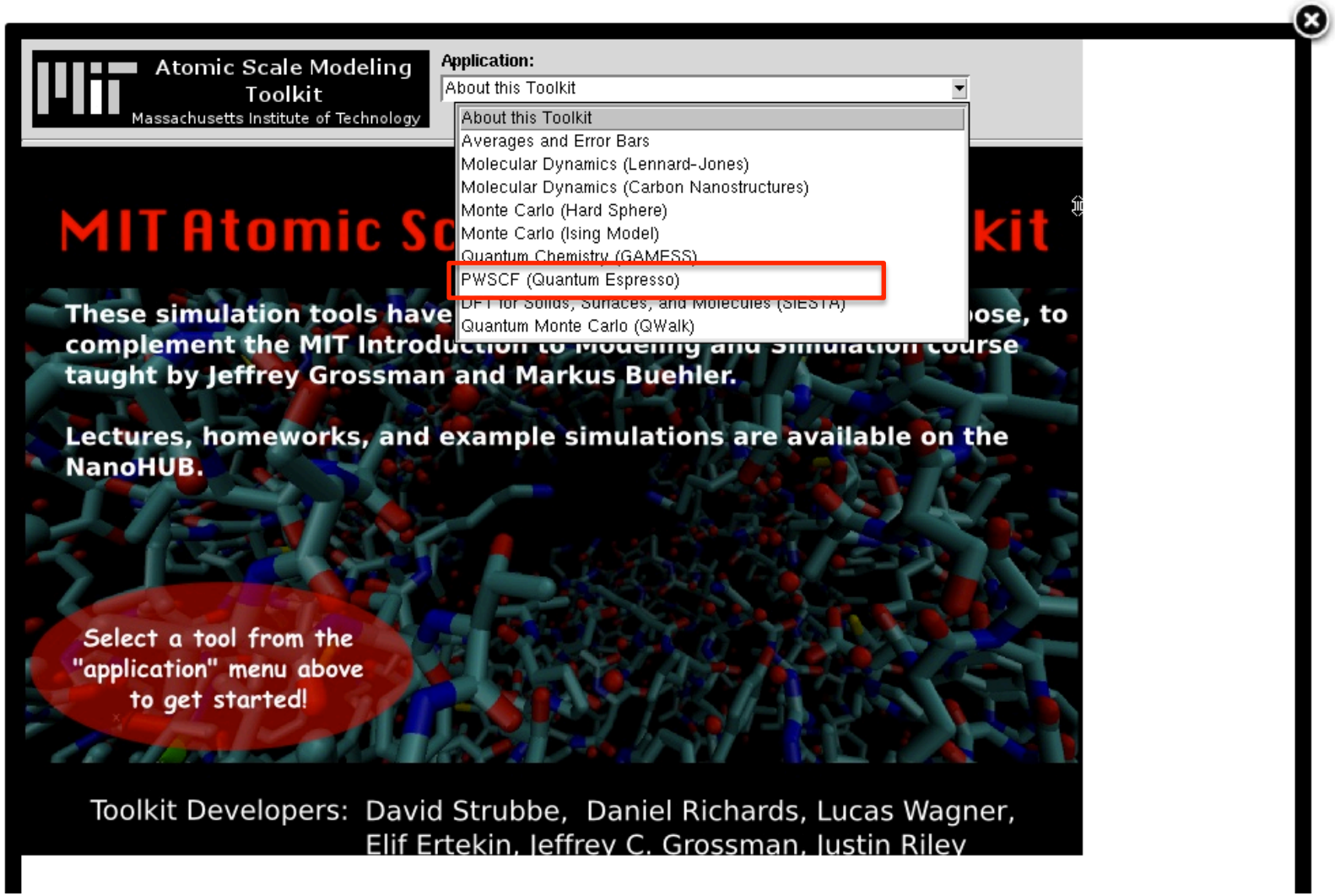
nanoHUB.org->Tools->MIT Atomistic Scale Modeling Toolkit



MIT Atomic Scale Modeling Toolkit



MIT Atomic Scale Modeling Toolkit



http://www.quantum-espresso.org/

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24.09.15

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20.06.15

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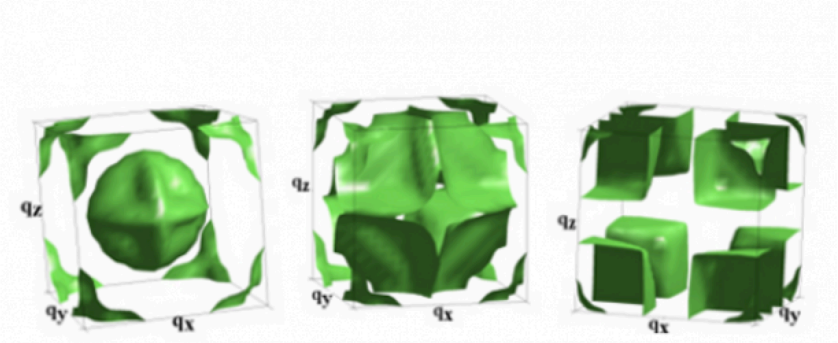


Phonons of SrTiO3 under strain, zero-frequency isosurface, Phys. Rev. Lett. 107, 257602 (2011) courtesy of T. Birol.

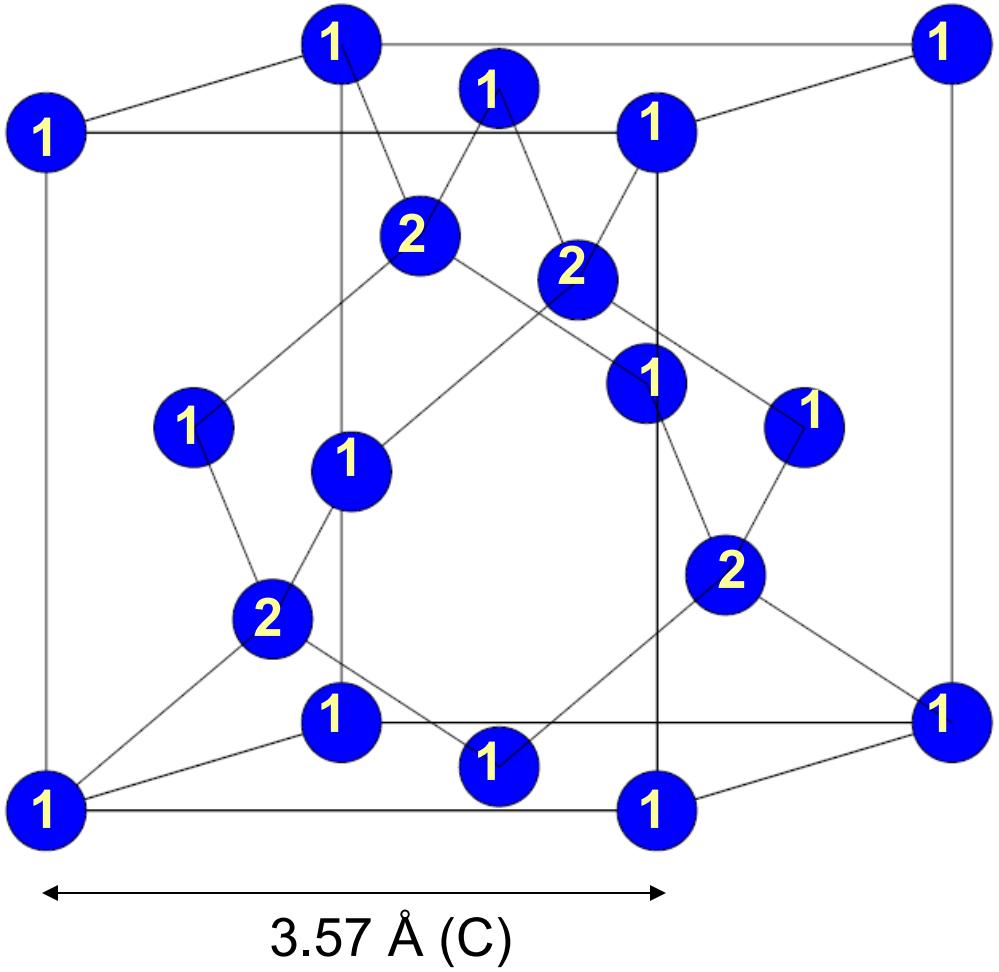
QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

READ MORE >

Diamond structure in PWSCF

ATOMIC_POSITIONS
C 0.00 0.00 0.00
C 0.25 0.25 0.25



1 Bohr = 0.529177249 Å

Application: PWSCF (Quantum Espresso)

1 Input → 2 Simulate

About this tool
Questions?

System | Atomic Coordinates | K Points | Looping | DOS | BANDS

Calculation: scf — SCF: self-consistent field calculation for converged charge densit

Bravais lattice: cubic F (face centered cubic)

Lattice constant: 7.5 — Units (in Bohr=0.529177249 Å)

Discussed later

Occupations: smearing

Smearing: gaussian

Degauss value: 0.07 — To do a spin-polarized calculation

Perform spin-polarized calculation?: no

Starting spin polarization: 0.0

Specify number of bands?: yes

Number of bands to calculate: 8

Wavefunction kinetic energy cutoff: 30.0 — Energy cut-off for plane waves (in Ry, 1 Ry = 13.6 eV)

Specify charge density cutoff?: yes

Charge density kinetic energy cutoff: 300.0 — Energy cut-off for charge density calculation

Specify FFT mesh for charge density?: yes

Convergence threshold: definition of convergence for charge density

Simulate >

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1 Input → 2 Simulate

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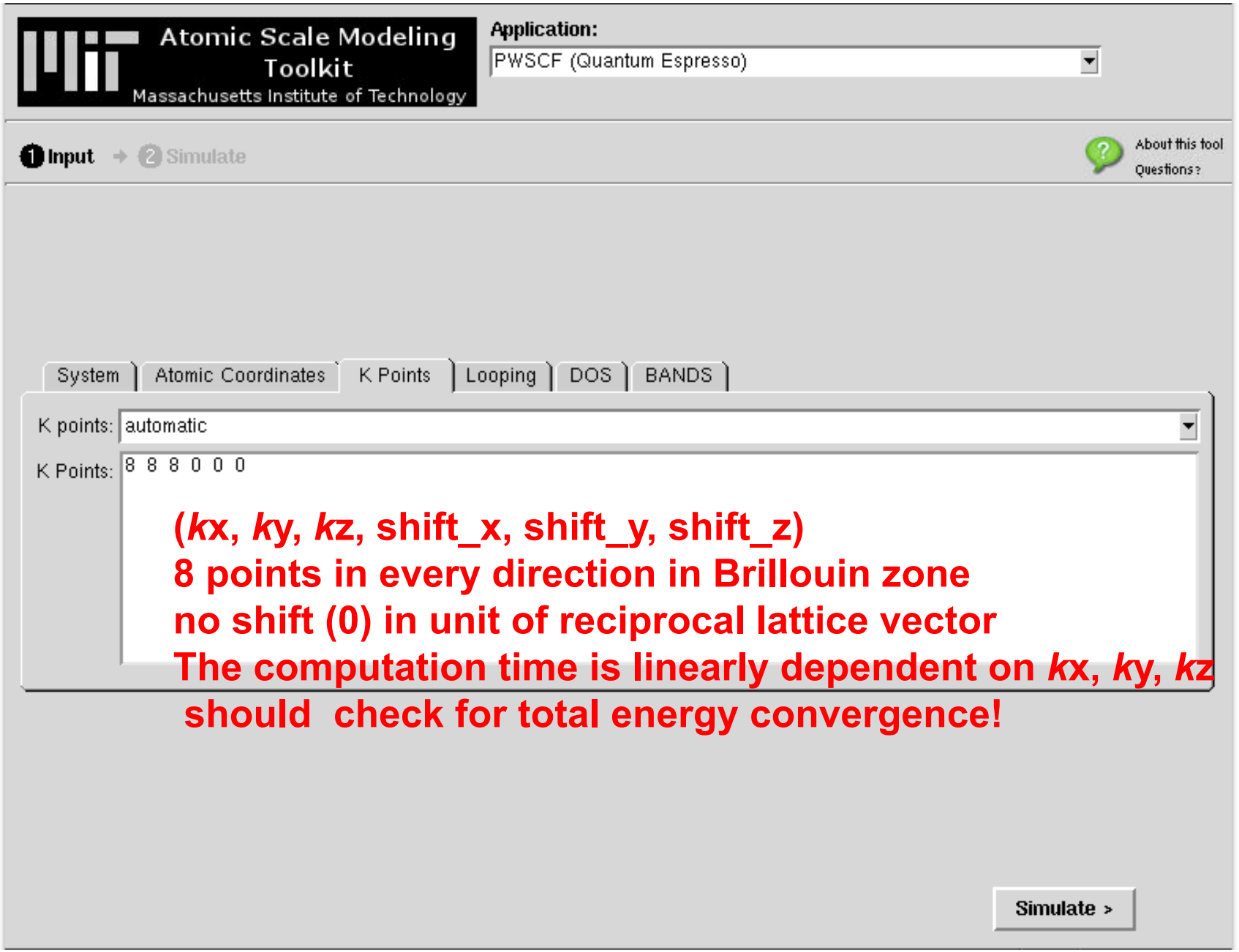
Coordinate units: alat

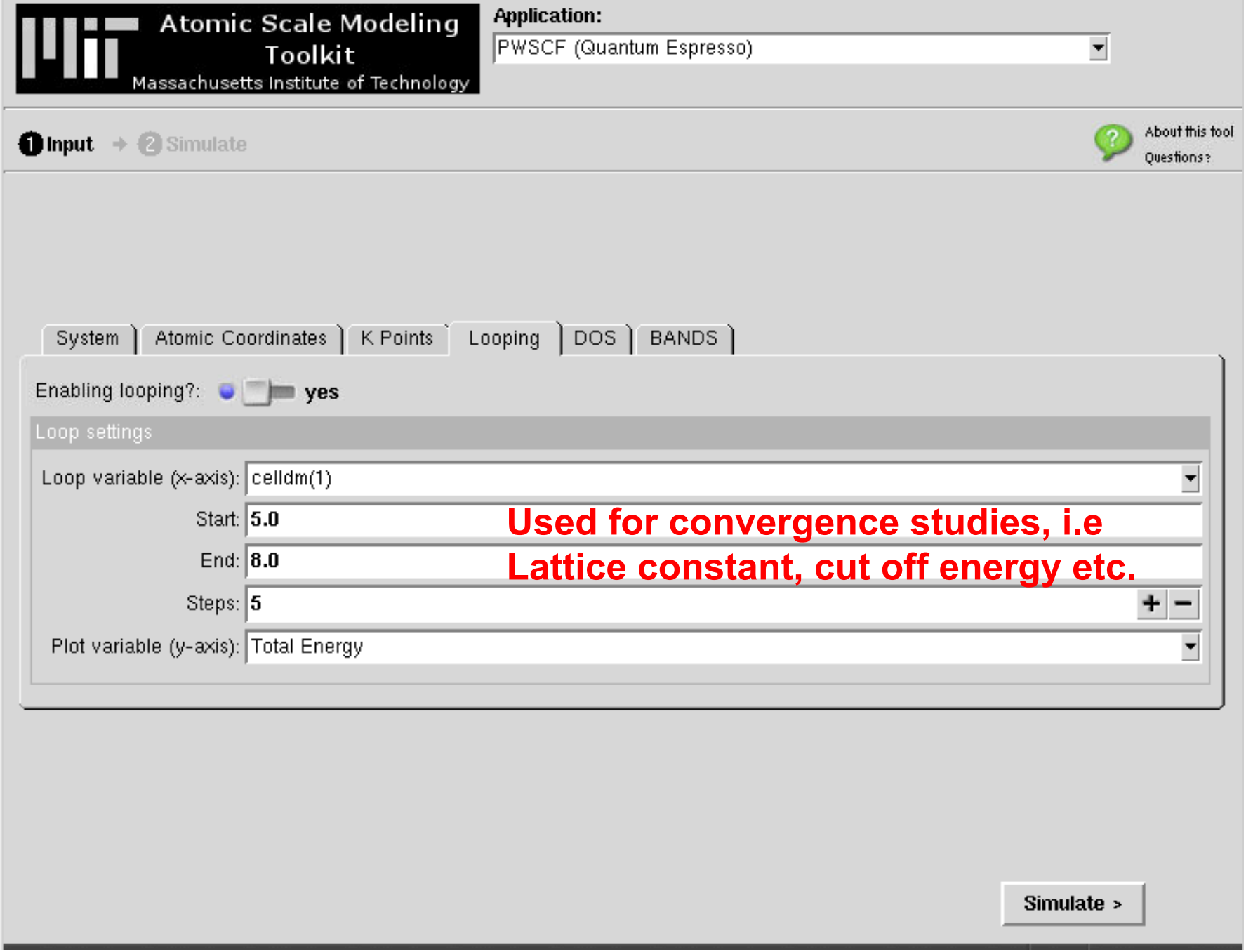
Atomic positions:

```
C  0.0  0.0  0.0
C  0.25  0.25  0.25
```

Atom type and atomic coordinates: Currently the toolkit has H, C, Al, Fe and Cu.

Simulate >


Atomic Scale Modeling Toolkit
Massachusetts Institute of Technology
Application:
PWSCF (Quantum Espresso)
1 Input
2 Simulate
About this tool
Questions?
System
Atomic Coordinates
K Points
Looping
DOS
BANDS
K points:
automatic
K Points:
8 8 8 0 0 0
(kx, ky, kz, shift_x, shift_y, shift_z)
8 points in every direction in Brillouin zone
no shift (0) in unit of reciprocal lattice vector
The computation time is linearly dependent on kx, ky, kz
should check for total energy convergence!
Simulate »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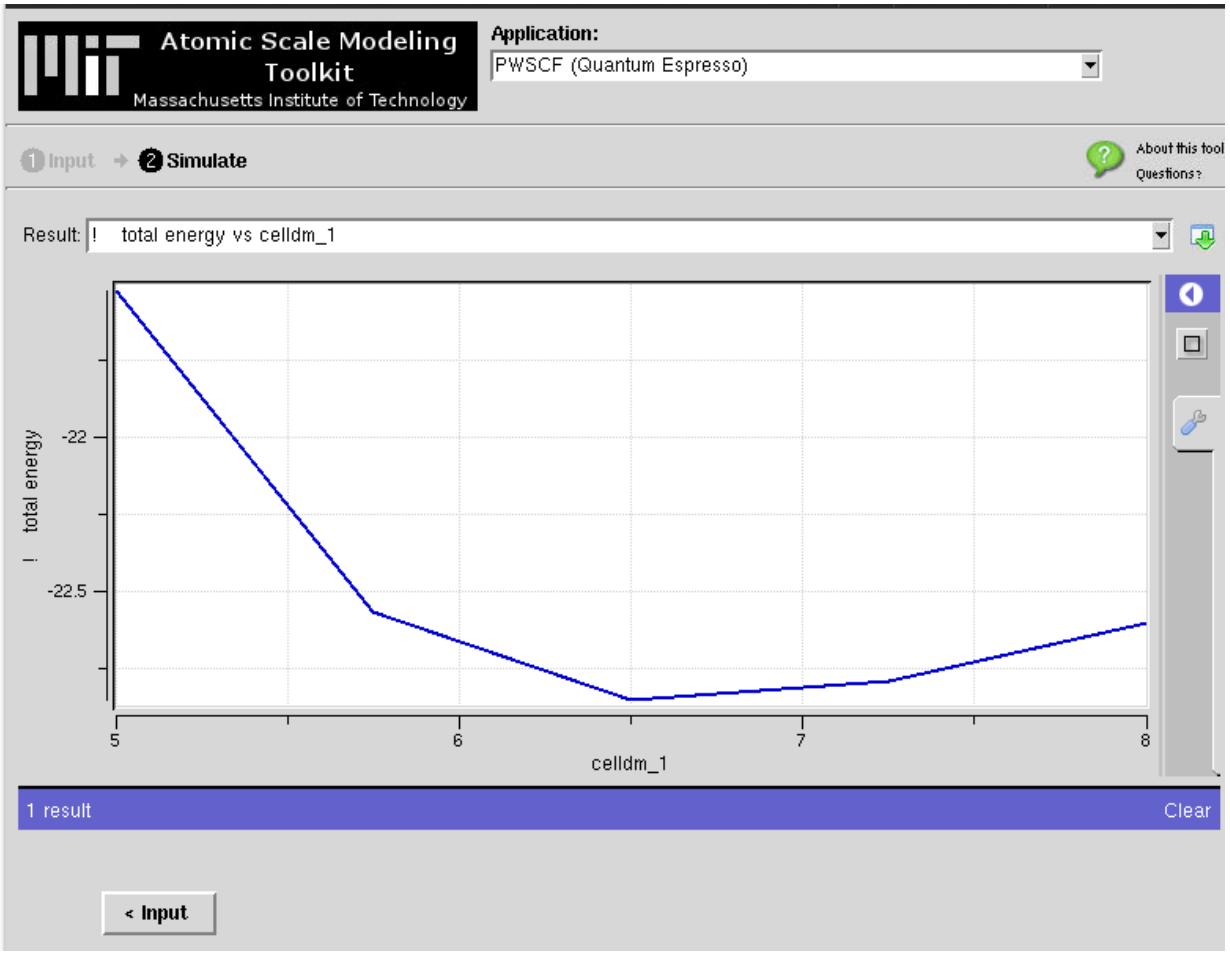
DOS
BANDS
Enabling looping?:
yes
Loop settings
Loop variable (x-axis):
celldm(1)
Start:
5.0
End:
8.0
Steps:
5
Plot variable (y-axis):
Total Energy
Used for convergence studies, i.e
Lattice constant, cut off energy etc.
Simulate »



Can compute:
Equilibrium lattice constant

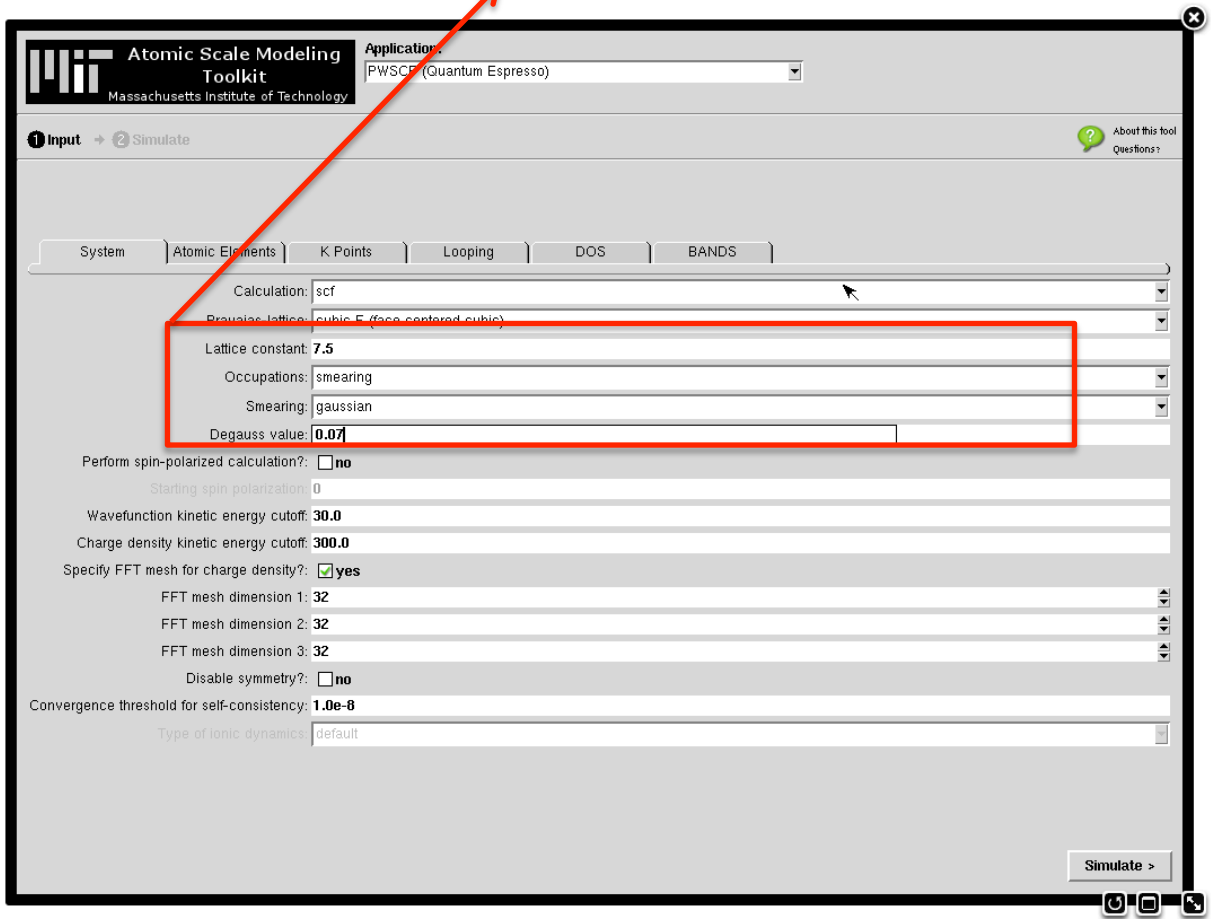
Units: Total energy (Ry) and celldm_1 (Bohr)

Example for metals (Aluminum, Cu)

Occupations: smearing — **define how electrons occupy the energy bands**

Smearing: gaussian — **method for 'smearing'**

Degauss value: 0.07 — **Gaussian distribution width for smearing**



For metals (such as Aluminum, copper), in order to determine the position of Fermi surface (maximum energy the electrons can reach, the finite numbers of electrons are filling orbitals from low energy to higher energy), we need some artificial gaussian type smearing function processing, and these three lines specify the method and parameters used.

Determine the equilibrium lattice constant