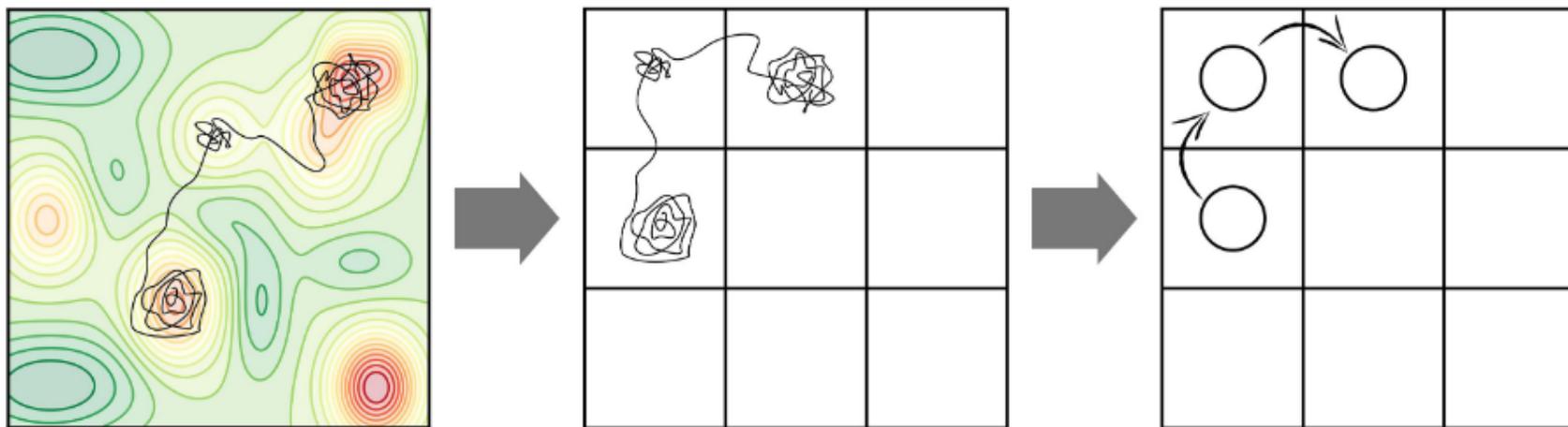


# LAMMPS

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Метод упругой ленты





**FIGURE 2 |** Coarse-graining of a molecular dynamics (MD) trajectory into a Markov chain. **(Left)** A possible MD trajectory (black) overlaid on the underlying potential energy surface (PES) of the system with red regions representing lower-energy basins. A large fraction of time is spent in these PES basins in vibrational motion around the respective minimum. At a certain moment in time, the systems finds an escape route to the next basin. **(Center)** Coarse-graining of PES minima into positions on a suitably defined lattice. Each lattice position represents the basin of attraction of a PES minimum. **(Right)** Coarse-graining of the continuous MD trajectory into a Markov chain of discrete hops between the basins/lattice positions.



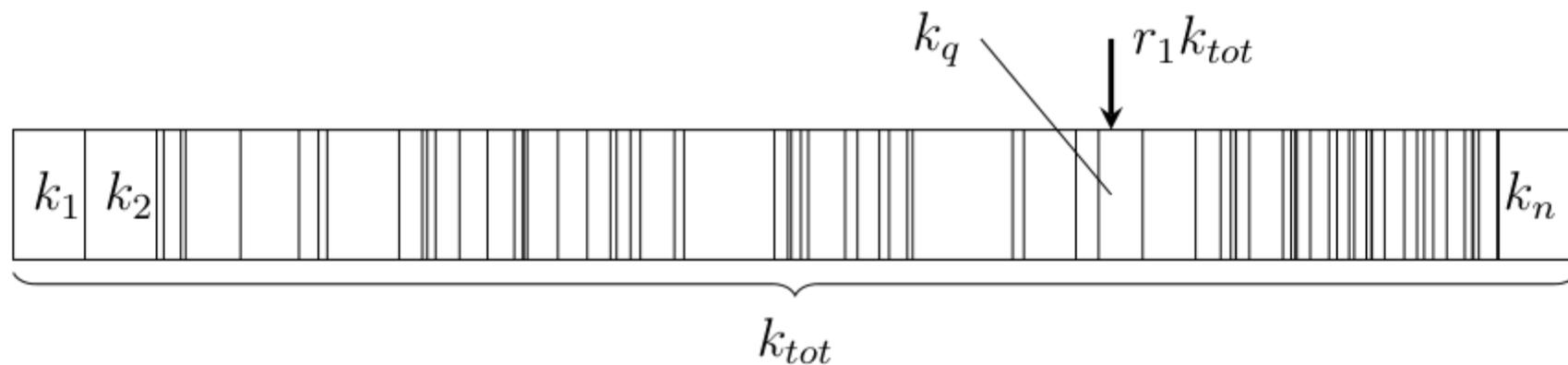
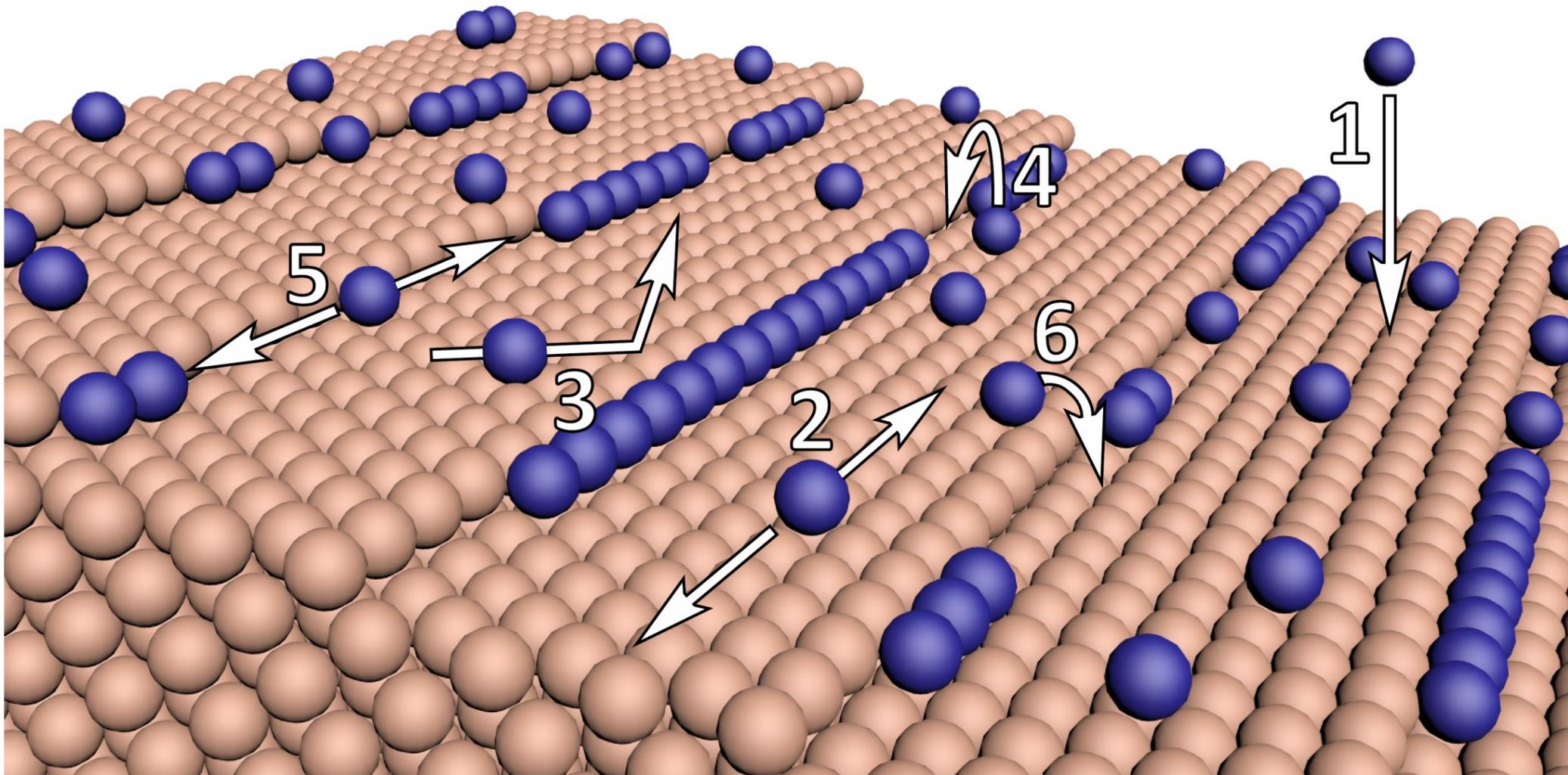
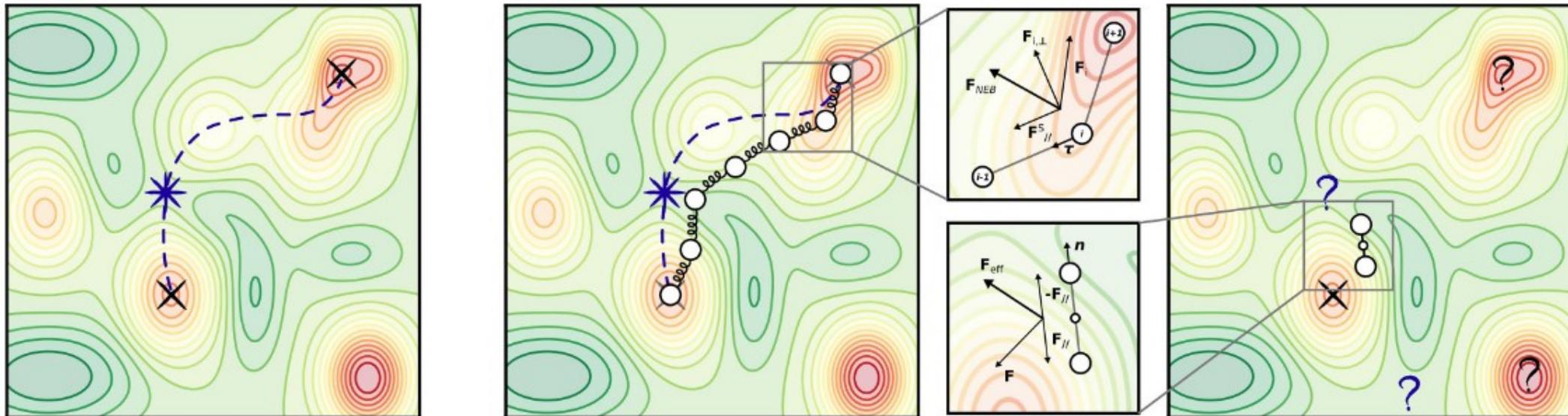


Рис. 2.5: Алгоритм случайного выбора состоявшегося события в кинетическом методе Монте-Карло на основании массива частот переходов



# Метод упругой ленты (NEB) и метод димера



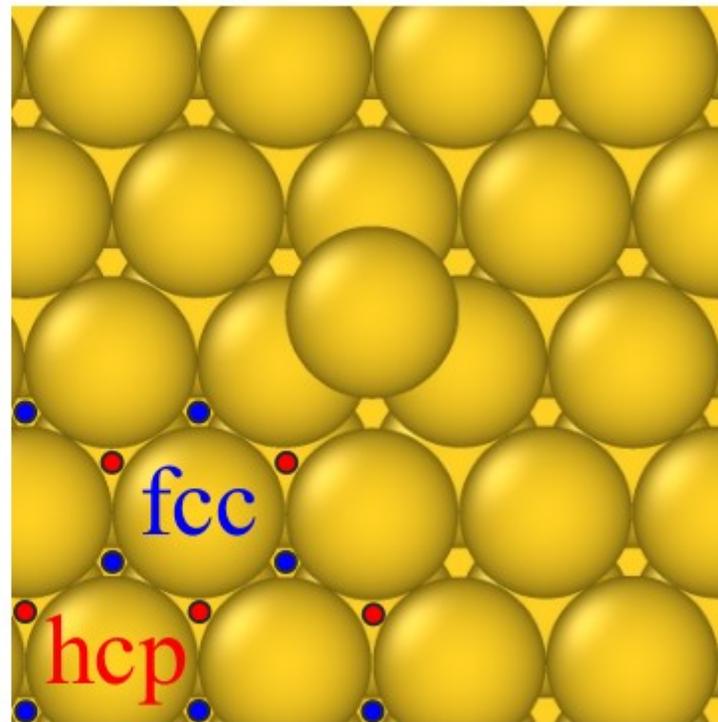
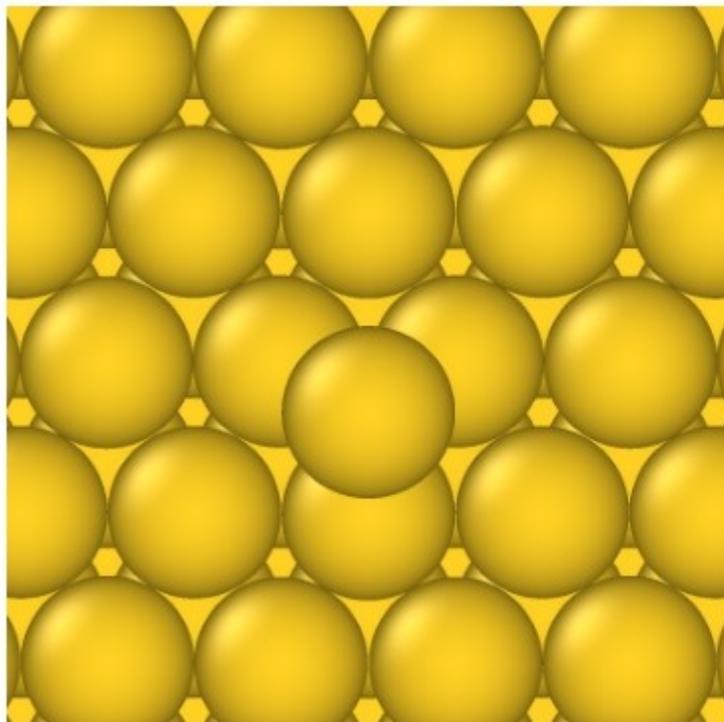
**FIGURE 5** | Transition states and most popular transition state (TS) search methods. **(Left)** An arbitrary PES exhibiting multiple minima (indicated by red colors). Black crosses mark two local minima, e.g., initial state (IS) and final state (FS) of a known elementary reaction. A violet star marks the location of the TS; a violet dashed line represents the minimum energy path connecting IS and FS. **(Center)** Illustration of the NEB method. The magnified panel shows the composition of forces which determines the effective NEB force acting on an image  $i$  at a certain optimization step. **(Right)** Illustration of the dimer method. The magnified panel shows the composition of forces which determines the effective force acting on the dimer at a certain optimization step, after the constrained minimization with respect to orientation.

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# Что делаем?

Ищем потенциальный барьер на Au(111) fcc  $\rightarrow$  hcp.



# Что делаем?

Ищем потенциальный барьер на Au(111) fcc  $\rightarrow$  hcp.

Для этого:

1. Создадим расчетную ячейку
2. Найдем равновесные начальное и конечное состояния
3. Натянем упругую ленту
4. Проанализируем результаты запуска

Запуск NEB с помощью LAMMPS на 8 процессорах

```
mpirun -np 8 lmp -partition 8x1 -var K 100 -in au-on-au.lmp
```

Запуск пачки задач по расчету NEB с помощью LAMMPS на 8 процессорах с помощью lammps-tools в менеджере очереди

```
export LAMMPS_PYTHON_TOOLS=/opt/lammps/tools/python/pizza  
parallel -j1 tsp archive_run.py -m "K={}" -- mpirun -np 8 lmp -partition  
8x1 -var K {} -in au-on-au.lmp ::: 1 10 100 1000
```