Zacros: case reports

Errors in the execution of Zacros 3.01 have been identified for several input conditions in the simulation of a particular system, tough the correct execution of example files.

The error message is:

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Internal error code 800001 from zacros_main: infeasible process in serial run!
This is a serious issue. Please notify the developers about this...

****

Using debug options lattice_handle_module reports errors when checking the lattice

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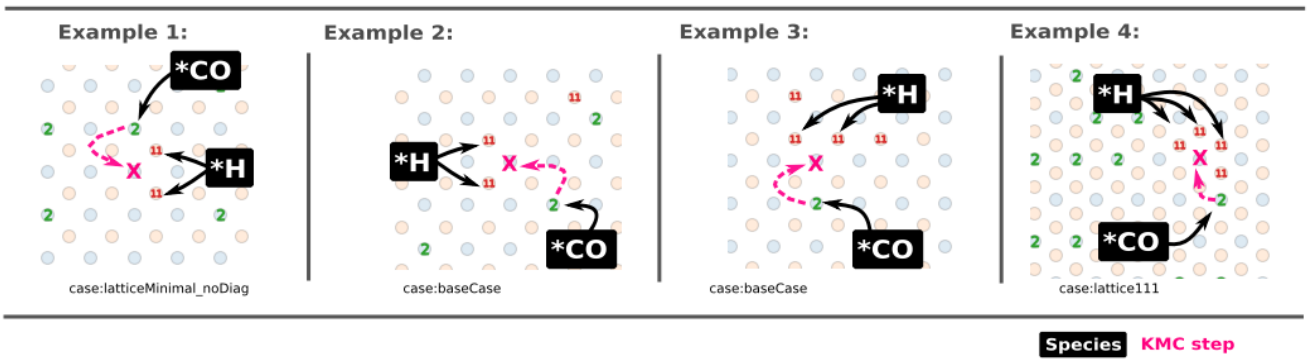
Internal error code 802001 from lattice_handle_module: invalid parity of adsorbspecposi and latticestate arrays.

More information:
Molecule numbering for lattice site 123 and molecule/entity 391 is inconsistent.

****

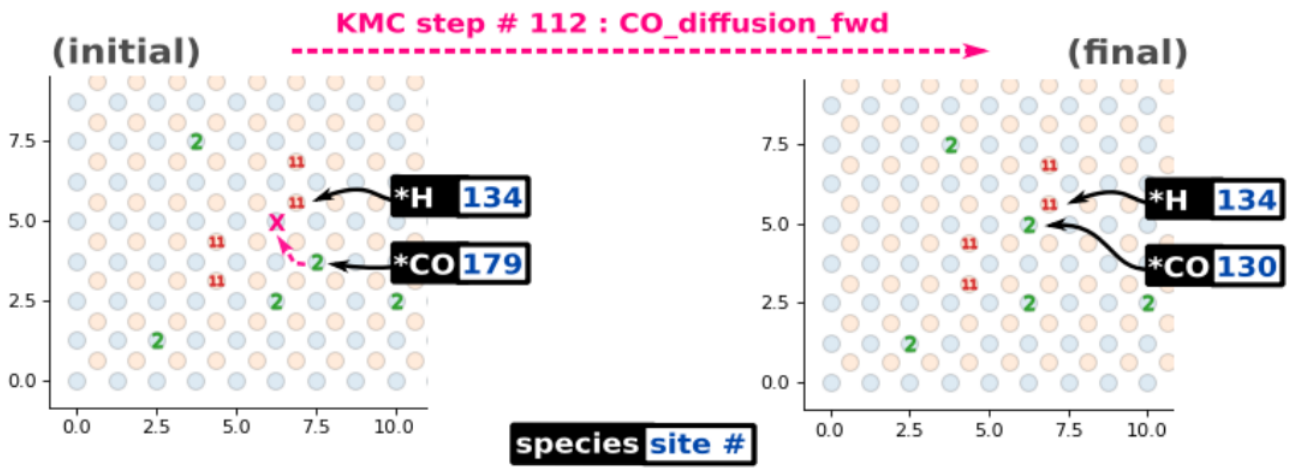
Similar errors are observed for zacros jobs in two separate HPC infraestructures and local installation. Errors appear as early as 50 KMC steps or much latter (>5000 KMC steps) deppending on the random seed used, no direct indication of memory shortage or memory leaks has been observed.

All error instances found so far have in common the insertion of an *CO species (labeled CO_N0) close to more than one *H species (labelled H_HrN0), may it be by CO adsorption or *CO diffusion (fwd or rev).



Nevertheless, CO-H interactions and reactive steps appear to be well defined and properly acknowledged in previous steps, moreover, in some instances similar local configurations were formed with identical input files (except the random seed) and proceeded without problems.
Some test for this error included simplifying the

Lets consider in detail a base case, in a correctly executed step:



From general_output.txt:

```
#line 1212:
 KMC step 112
  Elementary step CO_diffusion_fwd
  (...)
  involving site(s):      179    130
```

From globalenerg_debug.txt:

```
#line 1122:
 KMC step            112 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Cluster 21 was removed.            (removes previous *CO position, relabeled from cluster 21)
 Cluster 23 was relabeled to 21.
 Global-cluster 23 identified:      (adds new *CO position)
    Cluster number: 2
    Cluster description: CO_N0
    Mapping of lattice to pattern sites:  130
    Cluster graph-multiplicity: 1
    Its energy contribution is -1.54195940593633
 Global-cluster 24 identified:      (adds new *CO-*H interaction)
    Cluster number: 15
    Cluster description: CO-H-interaction
    Mapping of lattice to pattern sites:  130  134
    Cluster graph-multiplicity: 1
    Its energy contribution is 2.194567102947000E-003
 Current total lattice energy is -24.5541384625133
```

** Note that cluster 21 removed was previously cluster 24 (#line 1062) defined in:

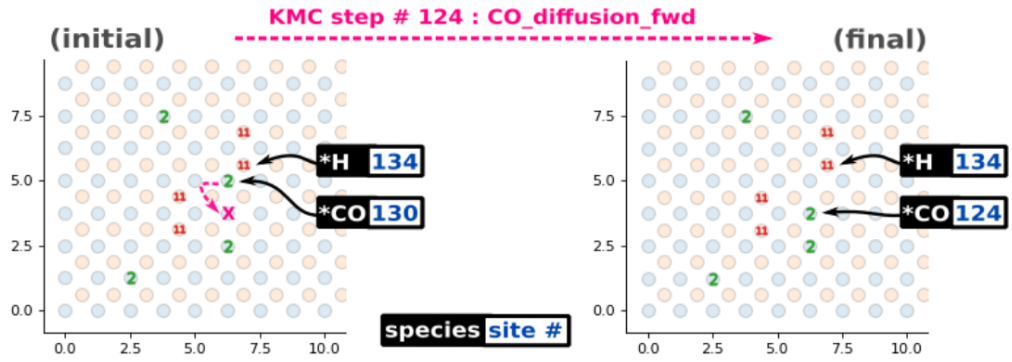
```
#line 1054:
 Global-cluster 24 identified:
    Cluster number: 2
    Cluster description: CO_N0
    Mapping of lattice to pattern sites:  179
    Cluster graph-multiplicity: 1
```

process_debug.txt includes (among many others)

```
#line 239451:Process 2910 identified:          (adds *CO+*H to *COH process to process list)
          Elementary step number: 5
```

Elementary step description: COH_formation_fwd
Mapping of lattice to pattern sites: 130 134
#line 239461:Process 2911 identified: **(adds *CO+*H to *HCO process to process list)**
Elementary step number: 9
Elementary step description: HCO_formation_fwd
Mapping of lattice to pattern sites: 130 134

In a later step the same *CO-*H interactions and events are properly removed:



From general_output.txt:

#line 1320:
KMC step 124
Elementary step CO_diffusion_fwd
occurred at time t = 3.808729530522180E-008
involving site(s): 130 124

From globalenerg_debug.txt:

#line 1246:
KMC step 124 ~~~~~~
Cluster 23 was removed. **(removes old *CO position, identified in step 112)**
Cluster 25 was relabeled to 23.
Cluster 16 was removed. **(removes old *CO-*H interaction, relabeled from cluster 24)**
Cluster 24 was relabeled to 16.
Global-cluster 24 identified: **(adds new *CO position)**
Cluster number: 2
Cluster description: CO_N0
Mapping of lattice to pattern sites: 124
Cluster graph-multiplicity: 1
Its energy contribution is -1.54195940593633
Current total lattice energy is -26.0982924355526

** Note that cluster 16 removed was previously labeled 24 (#line 1140) as defined in KMC step 112:
#line 1131:
Global-cluster 24 identified:
Cluster number: 15
Cluster description: CO-H-interaction
Mapping of lattice to pattern sites: 130 134
Cluster graph-multiplicity: 1
Its energy contribution is 2.194567102947000E-003

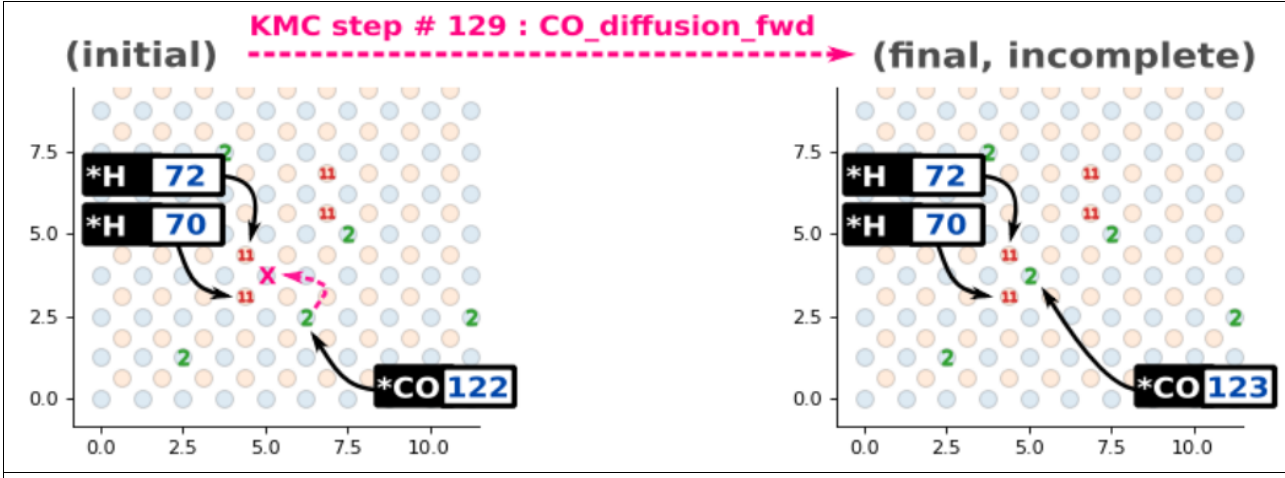
process_debug.txt includes (among may others)

#line 261316:Process 2786 was removed. **(removes *CO+*H to *COH process from process list)**
#line 261318:Process 2737 was removed. **(removes *CO+*H to *HCO process from process list)**
(...)
#line 262698:Process 2900 identified: **(adds*CO adsorption at site 130 to process list, implying 130 is now considered free)**
Elementary step number: 27

```
        Elementary step description: CO_ads_fwd
        Mapping of lattice to pattern sites:    130

** Processes relabeled:
line 239691: at KMC step 113, process 2910 (from KMC step 112) was relabeled to 2786.
line 239689: at KMC step 113, process 2911 (from KMC step 112) was relabeled to 2737.
```

The last step recorded in the base case is KMC step 129, a *CO difussion towards site. The last lattice snapshoot reported by zacros is the result of the previous KMC step 128.



From general_output.txt:

```
#line 1365:
 KMC step 129
   Elementary step CO_diffusion_rev
   occurred at time t = 3.893071641185187E-008
   involving site(s):      123    122
 (...)
```

From globalenerg_debug.txt:

```
#line 1304:
 KMC step            129 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Cluster 17 was removed.
 Cluster 25 was relabeled to 17.
 Global-cluster 25 identified:                    (adds new *CO position)
    Cluster number: 2
    Cluster description: CO_N0
    Mapping of lattice to pattern sites:  123
    Cluster graph-multiplicity: 1
    Its energy contribution is -1.54195940593633
 Global-cluster 26 identified:
    Cluster number: 15
    Cluster description: CO-H-interaction
    Mapping of lattice to pattern sites:  123   70     (adds new *CO-H interaction)
    Cluster graph-multiplicity: 1
    Its energy contribution is 2.194567102947000E-003
 Global-cluster 27 identified:                    (adds new *CO-H interaction)
    Cluster number: 15
   Cluster description: CO-H-interaction
    Mapping of lattice to pattern sites:  123   72
    Cluster graph-multiplicity: 1
    Its energy contribution is 2.194567102947000E-003
```

** Note that cluster 17 removed was previously labeled cluster 23 (#line 1095) as defined in KMC step 108:
#line 1131:
Global-cluster 23 identified:
Cluster number: 2
Cluster description: CO_N0
Mapping of lattice to pattern sites: 122
Cluster graph-multiplicity: 1
Its energy contribution is -1.54195940593633

From process_debug.txt

Remotion and relabeling of processes appear to proceed normally, for example:

Process identified in KMC step 127, line: 268863, diffusion away from initial *CO site(122)
Process 2919 identified:
Elementary step number: 23
Elementary step description: CO_diffusion_fwd
Mapping of lattice to pattern sites: 122 124

line 268959: at KMC step 128, process 2919 (from KMC step 127) was relabeled to 1513.
line 271625: at KMC step 129, process 1513 (from KMC step 127) was removed

that is, at the last KMC step (129) when a *CO diffuses from site 122 to site 123, a process for the *CO diffusion from its initial position (122) was removed.

However, no new processes were added when, for example, *CO+*H towards *HCO or *COH should be added for site pairs 122-70 and 122-72, also no new adsorption processes are added for site 123, which should count as an empty site now.