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Monitoring Chemical Reactions using On-the-Fly Molecular Species Analysis: fix reax/c/speceis

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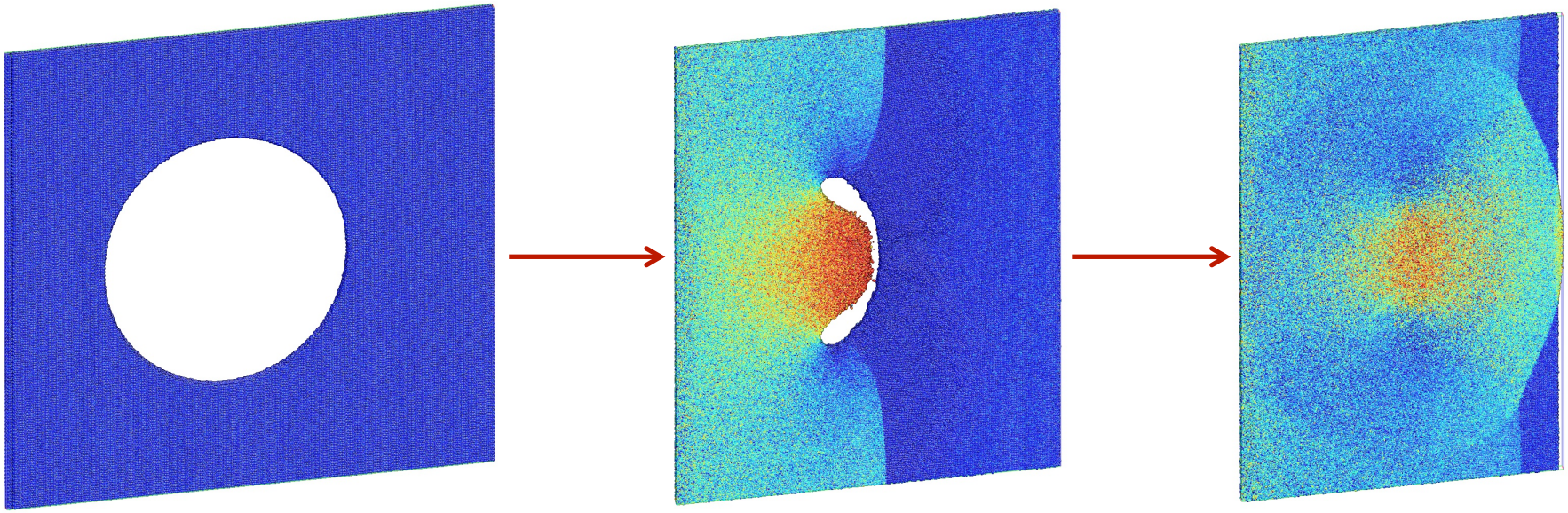
Motivation

- Very difficult to identify molecules and species in large-scale reactive simulations
- For example: Large-scale NEMD shock simulations using ReaxFF
  - Single crystal HNS ($C_{14}H_6N_6O_{12}$)
  - $2.2 \times 200 \times 175$ nm^3 with a 100 nm cylindrical void

142,324 HNS molecules

How many of what molecules?



0 ps

22 ps

36 ps

Motivation

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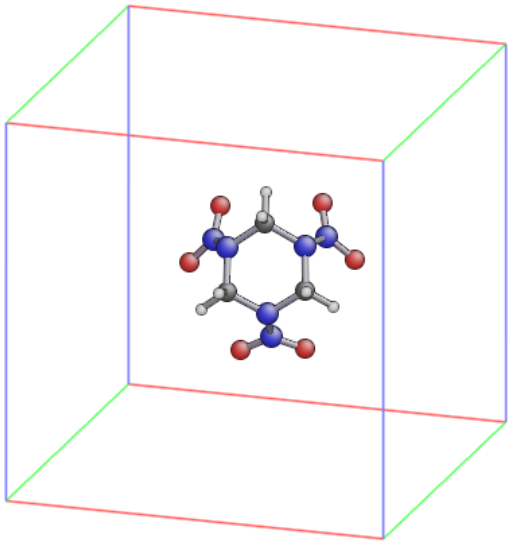
- Previous method with ReaxFF (using reax/c):
  - Use “fix reax/c/bonds” to print a connection table
  - Post-process the table with a serial program
  - Drawbacks:
    - Massive storage required
    - Time consuming post-process
    - No information on spatial distribution of molecules & species
- A new method with ReaxFF (using reax/c):
  - Avoids storing huge output files
  - Avoids post-processing with serial programs
  - Monitors molecules and species on-the-fly
  - Knows where and when specific molecules/species are formed
  - Currently limited to pair_style reax/c

Example

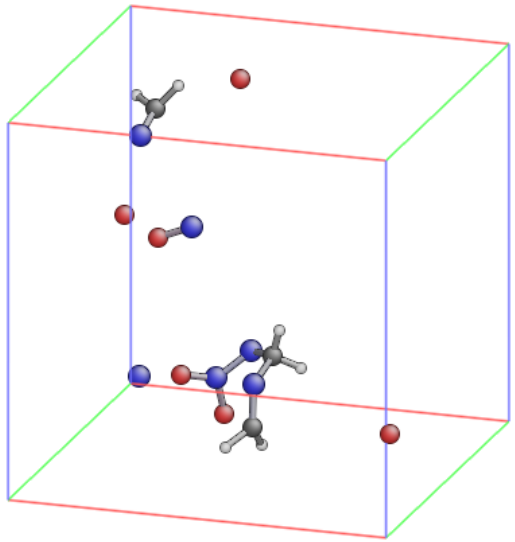
- Run $LAMMPS/examples/reax/in.reaxc.rdx
- A gas-phase RDX ($C_3H_6O_6N_6$) molecule looks like this:



  - Visualization using AtomEye over CFG files written by dump cfg command
    - dump 1 all cfg 100 *.cfg mass type xs ys zs
    - dump_modify 1 element C H O N
  - You can also use dump image, dump xyz, etc

Example

- Make the RDX molecule dissociate by adding thermal energy
  - velocity all create 2000.0 4712398
- Run for a 1000 steps
  - run 1000
- The RDX molecule becomes this:



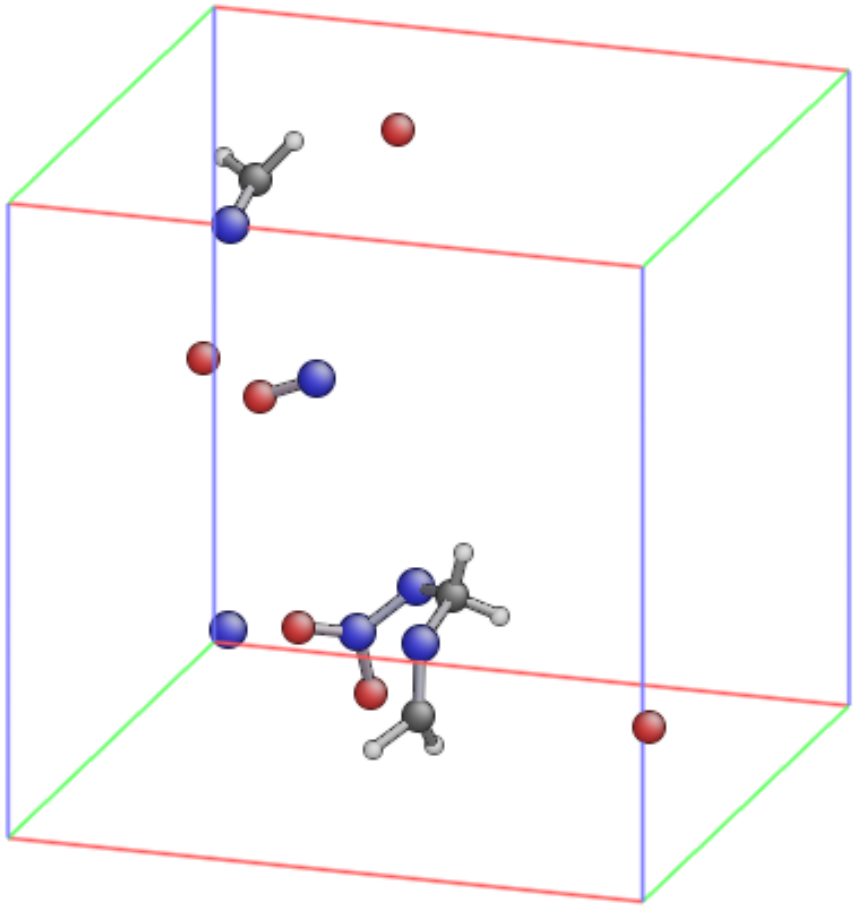
Example

- Identify number of molecules and species by adding the on-the-fly molecular species analysis command:
  - fix 3 all reax/c/species 1 10 100 species.out
  - The output file contains information on molecules and species

```
# Timestep     No_Moles     No_Specs     C3H606N6
100            1            1            1
# Timestep     No_Moles     No_Specs     C3H604N5       O2N
200            2            2            1              1
# Timestep     No_Moles     No_Specs     C3H604N5       O2N
300            2            2            1              1
# Timestep     No_Moles     No_Specs     C3H604N5       O2N
400            2            2            1              1
# Timestep     No_Moles     No_Specs     C3H604N5       O2N
500            2            2            1              1
# Timestep     No_Moles     No_Specs     C3H604N5       N        O
600            4            3            1              1        2
# Timestep     No_Moles     No_Specs     C3H604N5       N        O
700            4            3            1              1        2
# Timestep     No_Moles     No_Specs     C2H402N3       CH202N2  ON       O
800            4            4            1              1        1         1
# Timestep     No_Moles     No_Specs     C2H402N3       CH203N2  N        O
900            4            4            1              1        1         1
# Timestep     No_Moles     No_Specs     C2H402N3       CH2N     N        ON       O
1000           7            5            1              1        1         1        3
```

Example

# Timestep	No_Moles	No_Specs	C2H4O2N3	CH2N	N	ON	O
1000	7	5	1	1	1	3	



Input file: $LAMMPS/examples/reax/in.reaxc.rdx

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```
# ReaxFF potential for RDX system
# this run is equivalent to reax/in.reax.rdx

units           real

atom_style      charge
read_data       data.rdx

pair_style      reax/c control.reax_c.rdx
pair_coeff      * * ffield.reax C H O N

compute reax all pair reax/c

variable eb      equal c_reax[1]
variable ea      equal c_reax[2]
variable elp     equal c_reax[3]
variable emol    equal c_reax[4]
variable ev      equal c_reax[5]
variable epen    equal c_reax[6]
variable ecoa    equal c_reax[7]
variable ehb     equal c_reax[8]
variable et      equal c_reax[9]
variable eco     equal c_reax[10]
variable ew      equal c_reax[11]
variable ep      equal c_reax[12]
variable efi     equal c_reax[13]
variable eqeq    equal c_reax[14]

neighbor        2.5 bin
neigh_modify    every 10 delay 0 check no

fix             1 all nve
fix             2 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c

thermo          10
thermo_style    custom step temp epair etotal press &
                v_eb v_ea v_elp v_emol v_ev v_epen v_ecoa &
                v_ehb v_et v_eco v_ew v_ep v_efi v_eqeq

timestep        1.0

velocity        all create 2000.0 4712398

dump            1 all cfg 100 *.cfg mass type xs ys zs
dump_modify     1 element C H O N

fix             3 all reax/c/species 1 10 100 species.out

#dump           1 all atom 10 dump.reaxc.rdx

#dump           2 all image 25 image.*.jpg type type &
#               axes yes 0.8 0.02 view 60 -30
#dump_modify    2 pad 3

#dump           3 all movie 25 movie.mpg type type &
#               axes yes 0.8 0.02 view 60 -30
#dump_modify    3 pad 3

run             1000
```