

1 Variables

2 physical

| | var | symbol | documentation | type | units | eqs |
|----|-------------|----------------|-------------------------------------|--------|-----------------------------|-----------|
| 14 | r_{zN} | r_z | z-direction | frame | m | 10 |
| 13 | r_{yN} | r_y | y-direction | frame | m | 9 |
| 12 | r_{xN} | r_x | x-direction | frame | m | 8 |
| 11 | l_N | l | length | frame | m | |
| 18 | $n_{N,S}$ | n | fundamental state - molar mass | state | mol | |
| 24 | G_N | G | Gibbs free energy | state | $kg\,m^2\,s^{-2}$ | 18 |
| 16 | U_N | U | fundamental state - internal energy | state | $kg\,m^2\,s^{-2}$ | |
| 22 | H_N | H | Enthalpy | state | $kg\,m^2\,s^{-2}$ | 15 |
| 23 | A_N | A | Helmholts energy | state | $kg\,m^2\,s^{-2}$ | 17 |
| 15 | V_N | V | fundamental state - volume | state | m^3 | 11 |
| 17 | S_N | S | fundamental state - entropy | state | $kg\,m^2\,K^{-1}\,s^{-2}$ | |
| 25 | C_N | C | fundamental state - charge | state | $A\,s$ | |
| 20 | p_N | p | pressure | effort | $kg\,m^{-1}\,s^{-2}$ | 13 |
| 21 | $\mu_{N,S}$ | chemPot | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 14 |
| 19 | T_N | T | temperature | effort | K | 16 |

3 root

| | var | symbol | documentation | type | units | eqs |
|----|------------|------------|---------------------------------------|----------|-------|-----|
| 10 | $F_{N,A}$ | F | basic directed graph incidence matrix | network | | |
| 6 | t^e | te | time end | frame | s | 4 |
| 9 | Δ | pulse | pulse of length time interval | frame | | 7 |
| 4 | t | t | time | frame | s | |
| 7 | Δt | t_interval | time interval | frame | s | 5 |
| 5 | t^o | to | time zero | frame | s | 3 |
| 2 | 1 | one | numerical one | constant | | 1 |
| 1 | # | value | numerical value | constant | | |
| 3 | 0 | zero | numerical value zero | constant | | 2 |
| 8 | 0.5 | onehalf | numerical one half | constant | | 6 |

4 atomic

| | var | symbol | documentation | type | units | eqs |
|----|-------------|--------|-------------------------|----------|----------------|-----|
| 26 | λ_S | Mm | species' molecular mass | property | $kg\ mol^{-1}$ | |

5 Equations

6 Generic

| no | equation | documentation | layer |
|----|--|-------------------------------|----------|
| 1 | $1 := \text{Instantiate}(\#, \#)$ | numerical one | root |
| 2 | $0 := \text{Instantiate}(\#, \#)$ | numerical value zero | root |
| 3 | $t^o := \text{Instantiate}(t, 0)$ | time zero | root |
| 4 | $t^e := \text{Instantiate}(t, \#)$ | time end | root |
| 5 | $\Delta t := \text{Instantiate}(t, \#)$ | time interval | root |
| 6 | $0.5 := \text{Instantiate}(\#, \#)$ | numerical one half | root |
| 7 | $\Delta := \text{sign}(t - t^o) - \text{sign}(t - (t^o - \Delta t))$ | pulse of length time interval | root |
| 8 | $r_{xN} := \text{Instantiate}(l_N, \#)$ | x-direction | physical |
| 9 | $r_{yN} := \text{Instantiate}(l_N, \#)$ | y-direction | physical |
| 10 | $r_{zN} := \text{Instantiate}(l_N, \#)$ | z-direction | physical |
| 11 | $V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$ | volume | physical |
| 13 | $p_N := \frac{\partial U_N}{\partial V_N}$ | pressure | physical |
| 14 | $\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$ | chemical potential | physical |
| 15 | $H_N := U_N - p_N \cdot V_N$ | Enthalpy | physical |
| 16 | $T_N := \frac{\partial U_N}{\partial S_N}$ | temperature | physical |
| 17 | $A_N := U_N - T_N \cdot S_N$ | Helmholts energy | physical |

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| no | equation | documentation | layer |
|----|--|-------------------|----------|
| 18 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$ | Gibbs free energy | physical |