Changes to matflow tasks for DAMASK v3 alpha3

- Task: `generate_microstructure_seeds`
- Method: `random`
- Changes:

BEFORE

```yaml
- name: generate_microstructure_seeds
  method: random
  software: damask
  base:
    size: [1, 1, 1]
    grid_size: [16, 16, 16]
    num_grains: 4096
  output_map_options:
    phase_label: IF_steel
```

AFTER

```yaml
- name: generate_microstructure_seeds
  method: random
  software: damask
  base:
    size: [1, 1, 1]
    grid_size: [16, 16, 16]
    num_grains: 4096
    phase_label: IF_steel
```

Changes to matflow tasks for DAMASK v3 alpha3

- Task: `simulate_volume_element_loading`
- Method: `CP_FFT`
- Changes to hominization:

BEFORE

```
homogenization_schemes:
  SX:
    mech:
      type: none
```

AFTER

```
homogenization_schemes:
  SX:
    mechanical:
      type: pass
    N_constituents: 1
```

Changes to matflow tasks for DAMASK v3 alpha3

- Task: `simulate_volume_element_loading`
- Method: CP_FFT
- Changes to phases:

```
fcc  →  cF
bcc  →  cI
hcp  →  hP
```

BEFORE

```yaml
phases:
  IF_steel:
    lattice: bcc
    generic:
      output: [F, Fp, P, O]
    elasticity:
      type: Hooke
      C_11: 233.3e9
      …
    plasticity:
      type: phenopowerlaw
      output: [gamma_sl, xi_sl]
      N_sl: [12, 12]
      …
```

AFTER

```yaml
phases:
  IF_steel:
    lattice: cI
    mechanical:
      output: [F, F_p, P, O]
      elastic:
        type: Hooke
        C_11: 233.3e9
        …
      plastic:
        type: phenopowerlaw
        output: [gamma_sl, xi_sl]
        N_sl: [12, 12]
        …
```

Changes to matflow tasks for DAMASK v3 alpha3

- Task: `simulate_volume_element_loading`
- Method: CP_FFT
- Changes to output mapper:

BEFORE

```yaml
output_map_options:
  operations:
    - name: add_Cauchy
      args: {P: P, F: F}
      opts: {add_Mises: true}
    - name: add_strain_tensor
      args: {F: Fp, t: U, m: 0}
      opts: {add_Mises: true}
  incremental_data:
    - name: vol_avg_equivalent_stress
      path: constituent/1_IF_steel/generic/sigma_vM
      transforms: [mean_along_axes: 1]
      increments: 2
```

AFTER

```yaml
output_map_options:
  operations:
    - name: add_stress_Cauchy
      args: {P: P, F: F}
      opts: {add_Mises: true}
    - name: add_strain
      args: {F: F_p, t: U, m: 0}
      opts: {add_Mises: true}
  incremental_data:
    - name: vol_avg_equivalent_stress
      path: constituent/IF_steel/generic/sigma_vM
      transforms: [mean_along_axes: 1]
      increments: 2
```

Changes to matflow tasks for DAMASK v3 alpha3

- Task: `simulate_volume_element_loading`
- Method: `CP_FFT`
- Additions to output mapper:

```yaml
output_map_options:
  volume_data:
    - field_name: sigma
      out_name: vol_avg_stress
      transforms: [mean_along_axes: 1]
      increments:
        - values: [10, 20]
  phase_data:
    - field_name: sigma
      phase_name: IF_steel
      out_name: phase_avg_stress
      transforms: [mean_along_axes: 1]
      increments:
        - step: 2
  field_data:
    - field_name: sigma
      increments:
        - values: [10, 20]
    - field_name: grain
    - field_name: phase
  grain_data:
    - field_name: sigma
      increments:
        - start: 10
        - stop: 20
        - step: 2
```

Changes to matflow tasks for DAMASK v3 alpha3

- Task: `simulate_volume_element_loading`
- Method: `CP_FFT`
- Translating an `incremental_data` block to a `phase_data` block:

BEFORE

```yaml
output_map_options:
  incremental_data:
    - name: phase_avg_stress
      path: constituent/1_IF_steel/generic/sigma
      transforms: [mean_along_axes: 1]
      increments: 2
```

AFTER

```yaml
output_map_options:
  phase_data:
    - field_name: sigma
      phase_name: IF_steel
      out_name: phase_avg_stress
      transforms: [mean_along_axes: 1]
      increments:
        - step: 2
```

Changes to matflow tasks for DAMASK v3 alpha3

Summary

- **generate_microstructure_seeds-random**
  - phase_label and orientation_coordinate_system move from output map options to inputs

- **simulate_volume_element_loading-CP_FFT**
  - Changes to homogenisation, phases for mat file
  - Changes to names of operations in output map of VE sim (add_stress_Cauchy, add_strain)
  - Phases in hdf file don’t have 1_ at start anymore
  - Fe, Fp, Fi, Lp, Li changed to F_e, F_p, F_i, L_p, L_i

- VE grains are now indexed from 0 not 1