Accelerating multi-scale microstructure simulations by exploiting local macroscopic quasi-homogeneities

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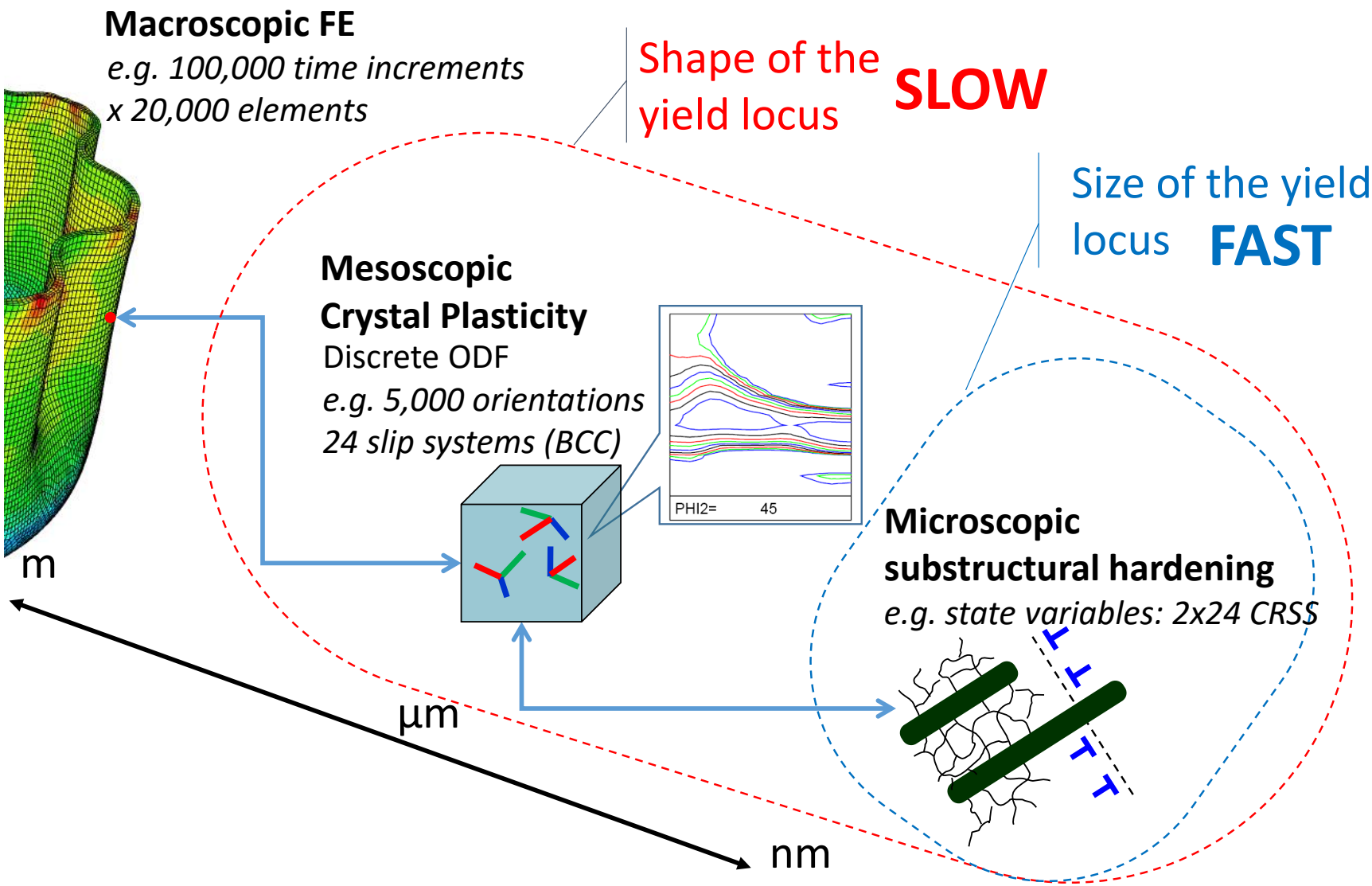
Outline of the HMS modelling framework



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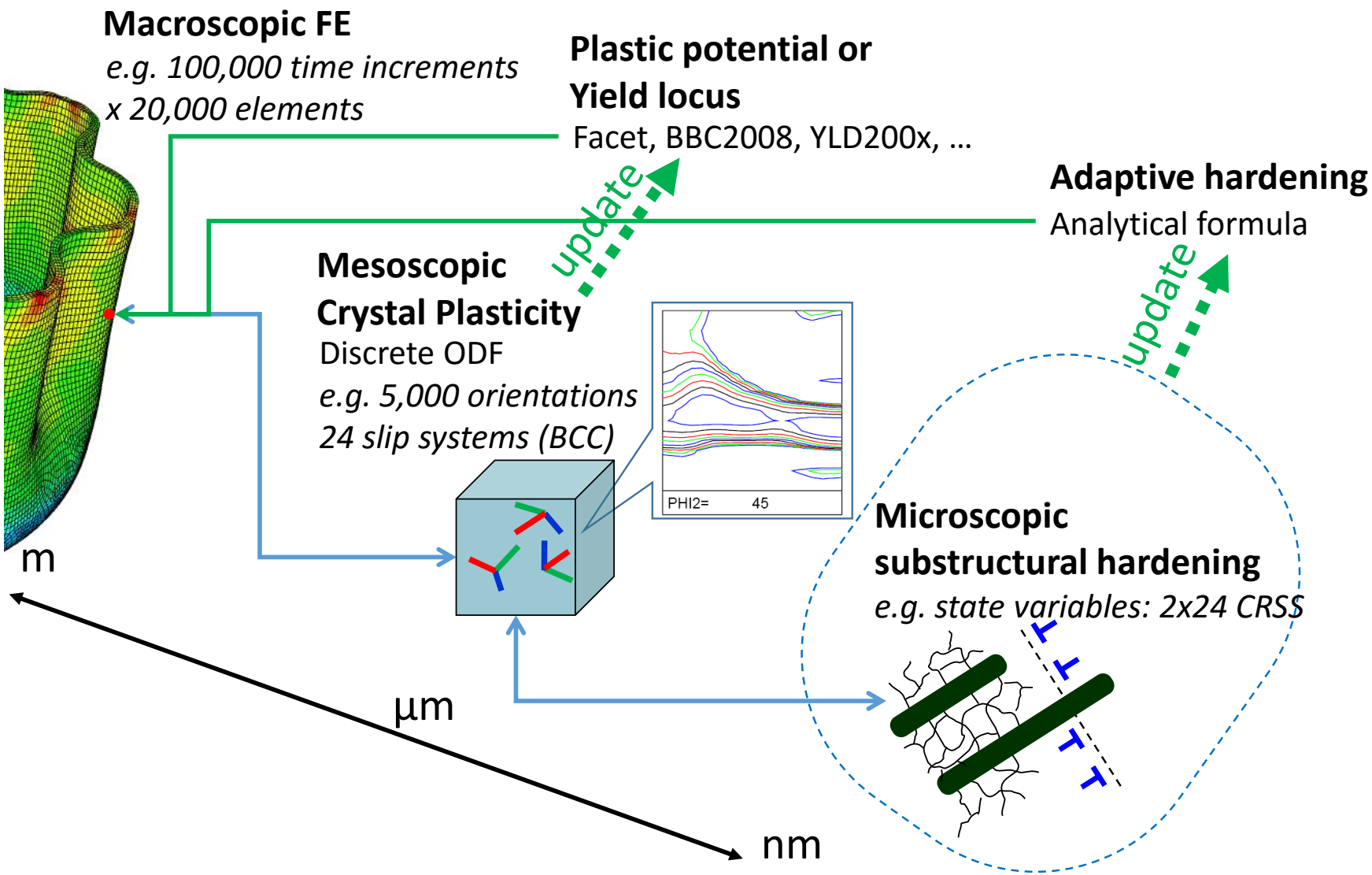


Computational advantage of the HMS

How much can we save in terms of the simulation time?

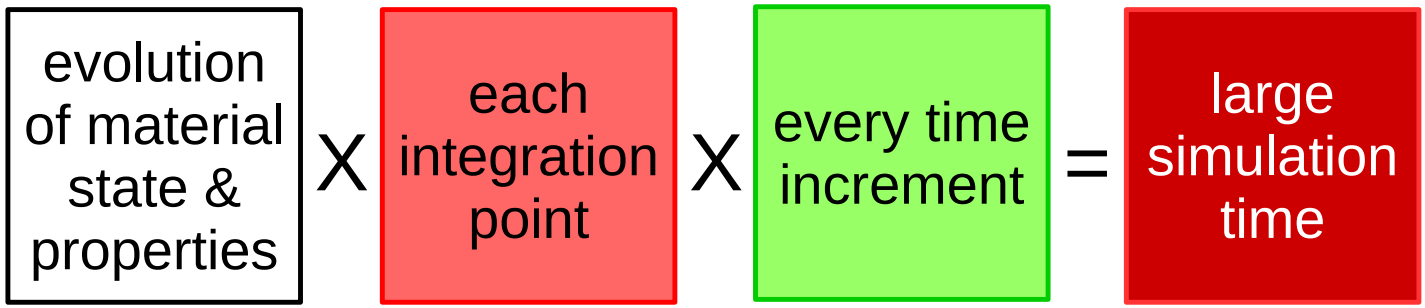
For example:
Crystal Plasticity fully embedded in an explicit time integration FE:

- 1 call/update to the fine-scale CP model per increment of the coarse-scale FE model

$t_{CPFEM} \approx 100.000\,\text{updates} \times 20.000\,\text{integration points} \times t_{CP} + t_{FE}$

HMS: Crystal Plasticity hierarchically coupled with FEM:
$t_{HMS} \approx 30\,\text{updates} \times 20.000\,\text{integration points} \times t_{CP} + t_{FE}$

Contributions to the computational cost of multi-scale CP-FEM



The HMS addresses the issue:

- in the temporal dimension: reconstruction of the plastic potential function is adaptively conducted only at the moments when a given deformation-based criterion is satisfied.
- in the spatial dimension: another acceleration is possible!

Acceleration of the multi-scale CP models by exploiting spatial quasi-homogeneities

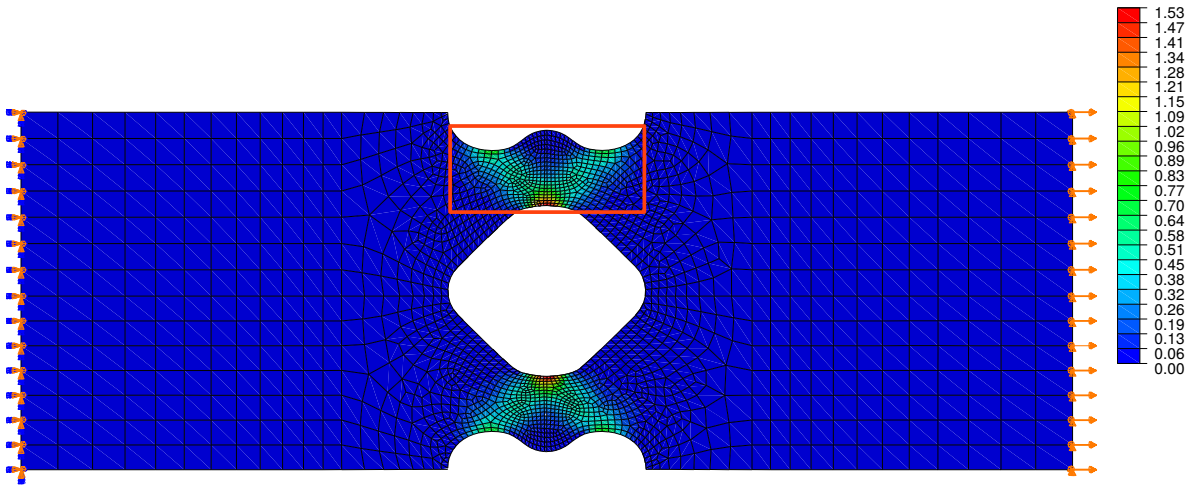
Fundamental assumptions:

- Similar microstructural state variables subjected to a similar deformation history would evolve along nearly identical trajectories.
- Derived macroscopic plastic properties would be similar as well.

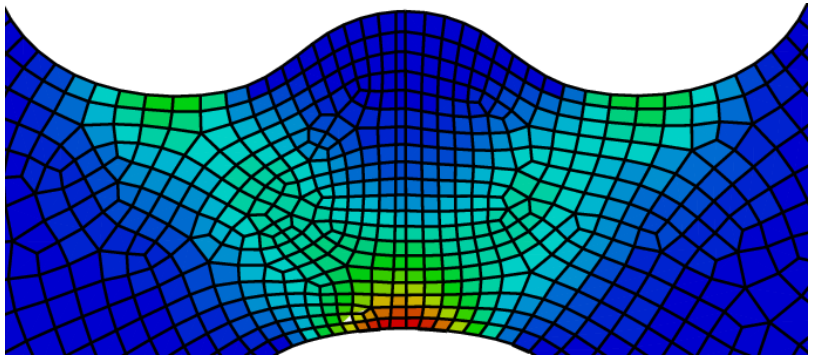
Additional assumption:

- The accumulated plastic strain determines the evolution of the material properties.

Example:
field of total
plastic slip

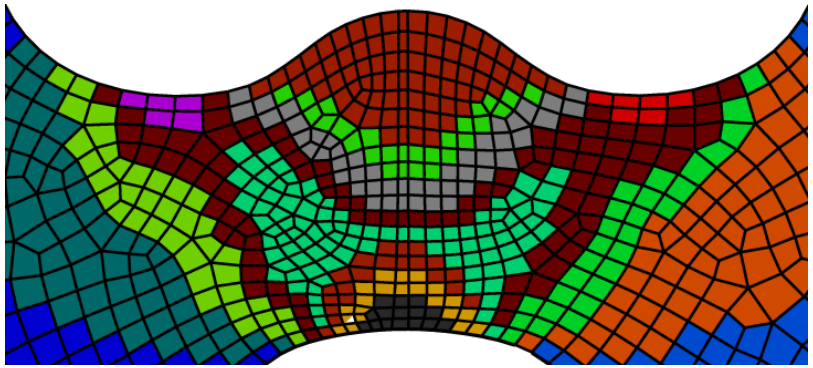


Exploiting spatial quasi-homogeneities



control field variables: *total plastic slip*, *accumulated plastic strain*, *equivalent plastic strain* . . .

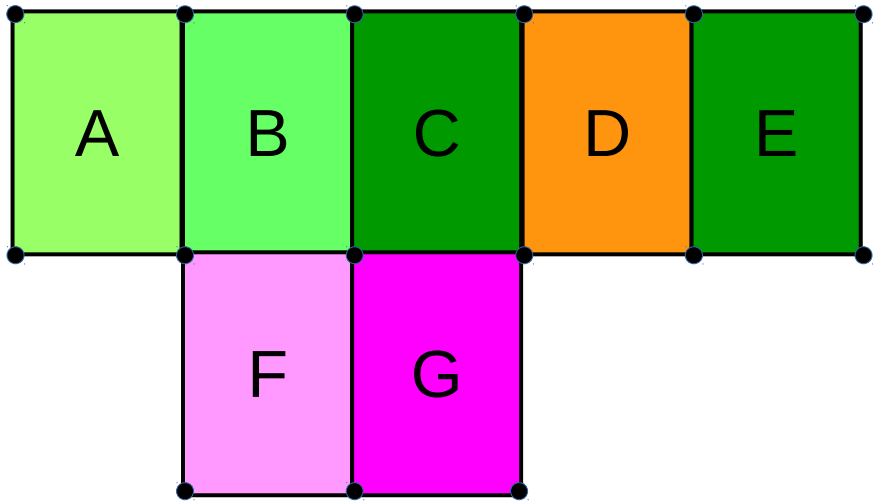
Integration points grouped together (clustered):



material state: *microstructure (texture, substructure, . . .), plastic potential function, . . .*

material properties: *plastic potential function, hardening, . . .*

Overview of the spatial clustering method in HMS



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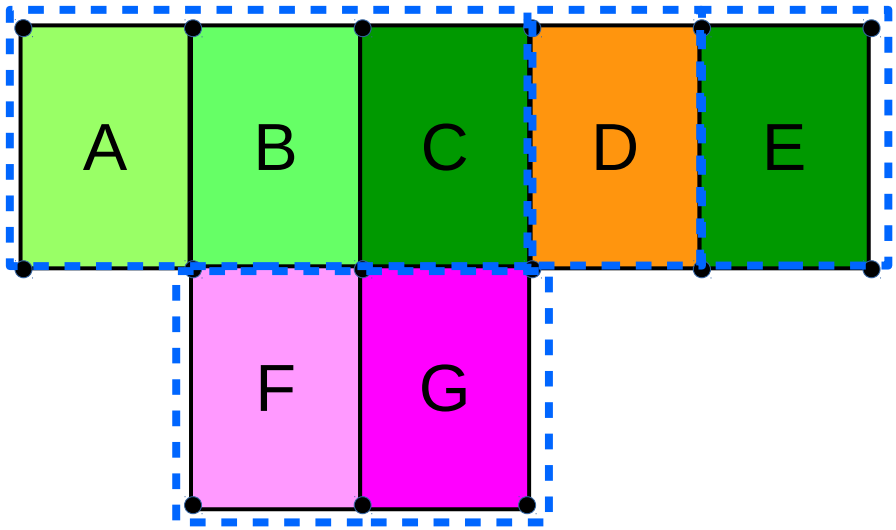

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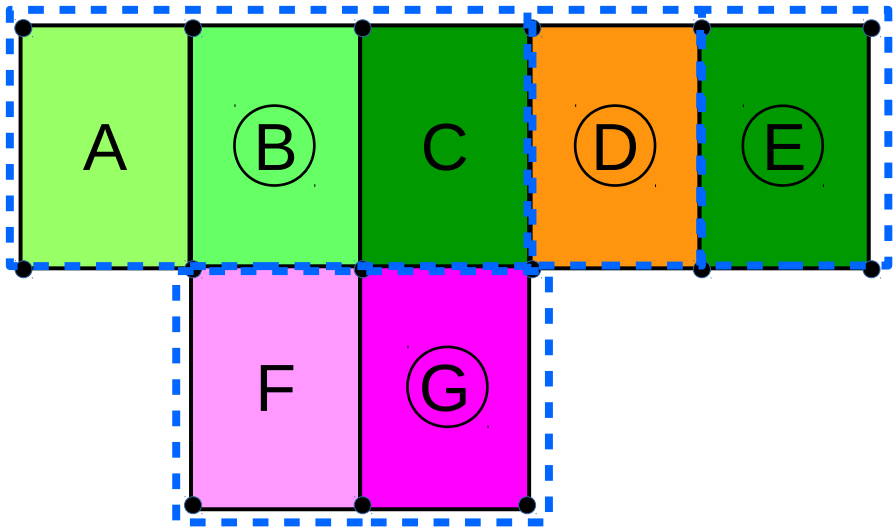

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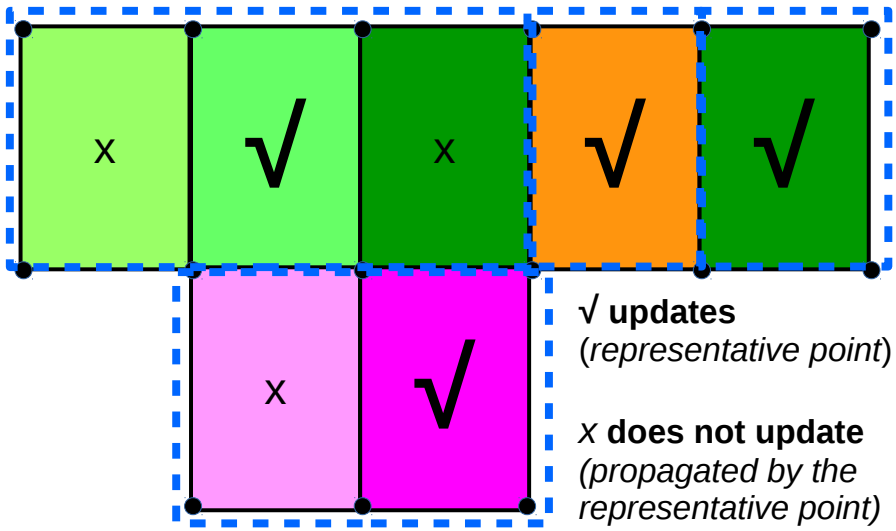


But it has to be decided when and how the clusters should be formed.

Clustering schemes and clustering criteria

Clustering scheme decides when the clusters are formed.
Several schemes can be considered, including:

1. **static**: the clusters are constructed once and later used throughout the simulation.
2. **dynamic**: the cluster are adaptively rebuilt as the HMS simulation advances.

Clustering criterion decides how the integration points are grouped into the clusters.

- primary criterion: spatial proximity of the integration points
- secondary criteria:
  1. magnitude of total plastic slip, or
  2. plastic strain tensor,
  3. sum of the absolute values of plastic strain increment tensors,
  4. ...

Static spatial clustering

The algorithm in a nutshell:

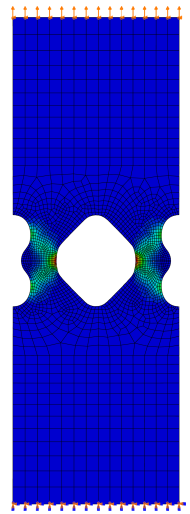
- Parameter: number of clusters k.
- Initialization: all integration points belong to a single cluster
- Given the control field variable and the Euclidean distance matrix, construct k clusters and use these clusters throughout the simulation.

The inputs may be taken from:

- a plain FE simulation (non-HMS) of the process (off-line), or
- the HMS simulation itself, for instance when the first update of properties is calculated (on-line)
- a reference HMS simulation (off-line, very impractical)

Static spatial clustering in HMS: performance gain vs accuracy

Example: tensile test on a complex geometry specimen

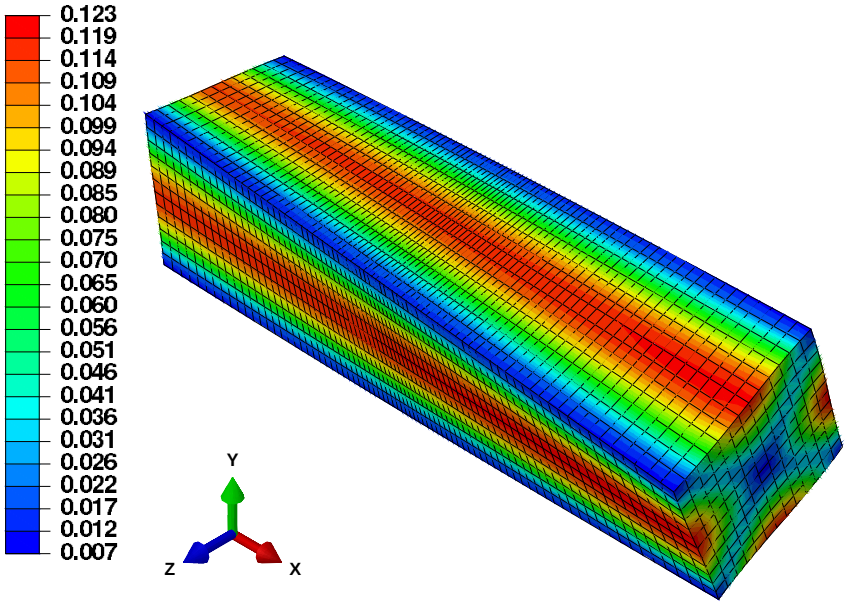


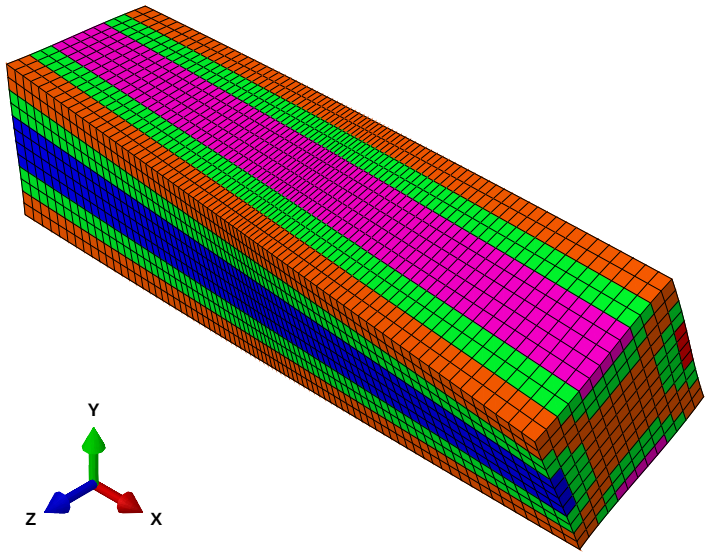
$$\text{speedup}(\#\text{clusters}) = \frac{t_{HMS}}{t_{HMS,\#clusters}}$$

Note: the deformation is nearly monotonic in this example.

Static spatial clustering in HMS

Example: torque bar, 9 clusters

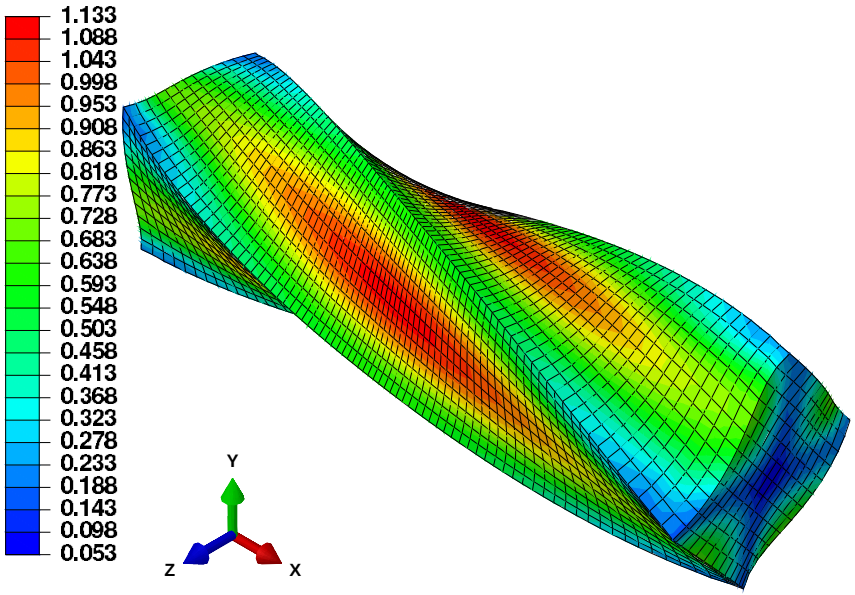


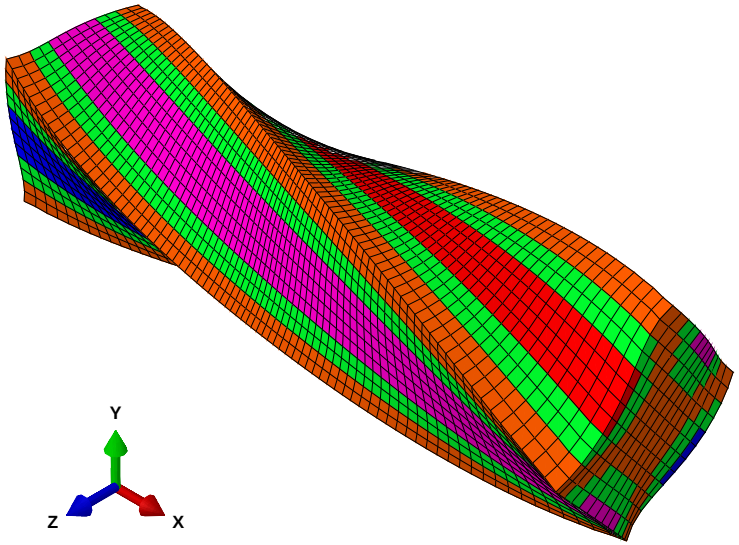


- Example: a bar subjected to torsion followed by tension.
- The two deformation steps introduce a non-monotonic strain path.

Static spatial clustering in HMS

Example: torque bar, 9 clusters





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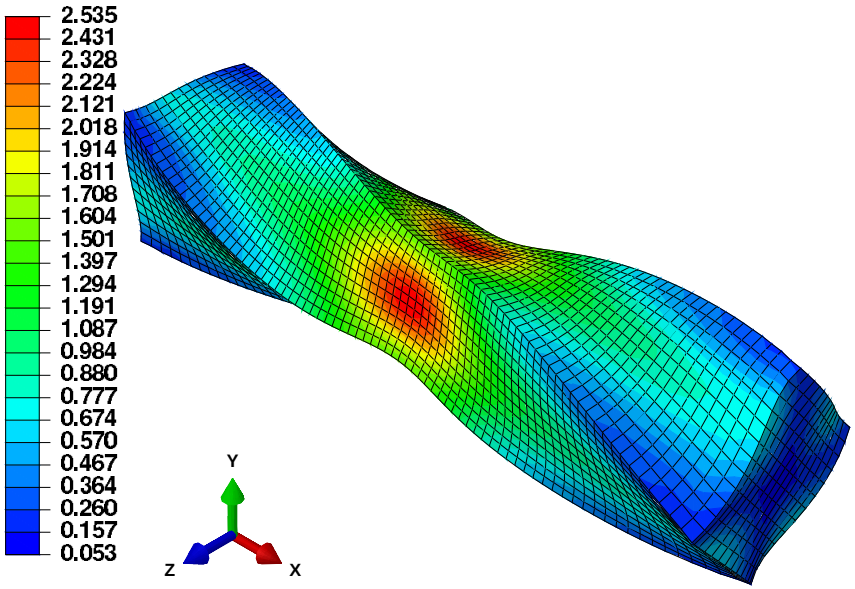

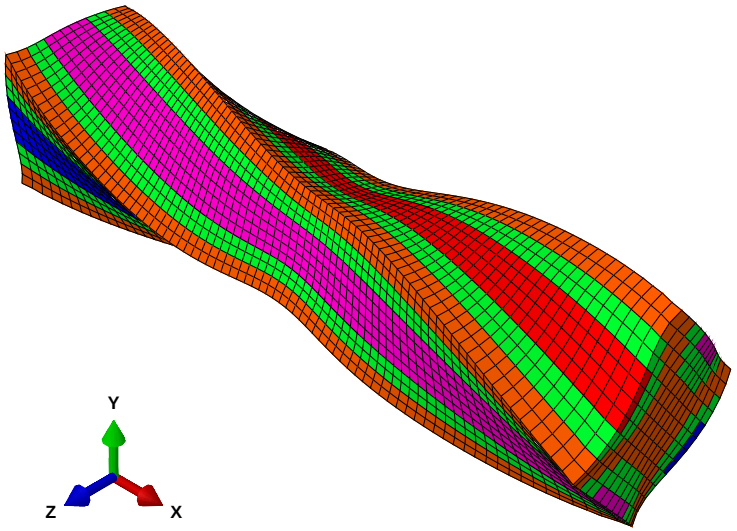

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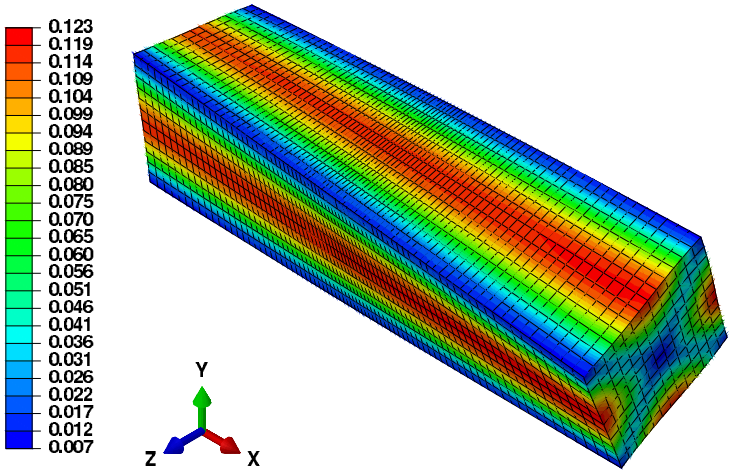
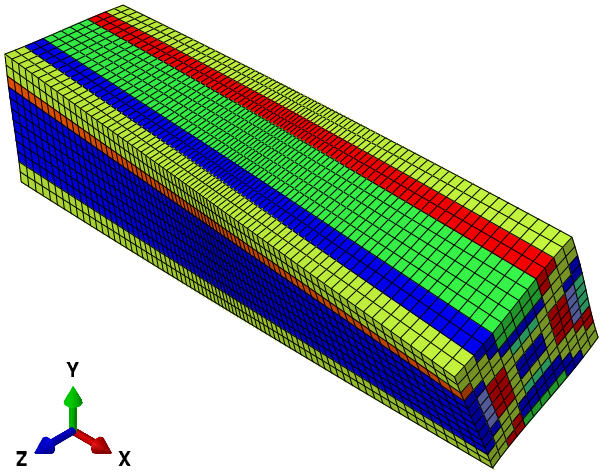
Static spatial clustering in HMS

Example: torque bar, 27 clusters





Static spatial clustering in HMS

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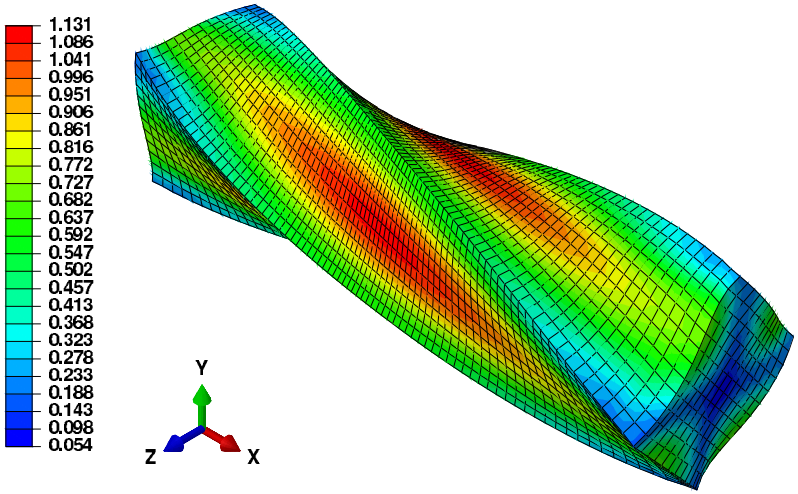

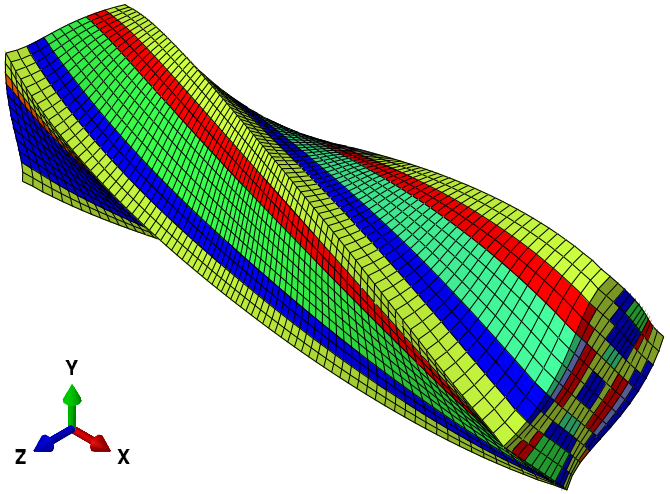

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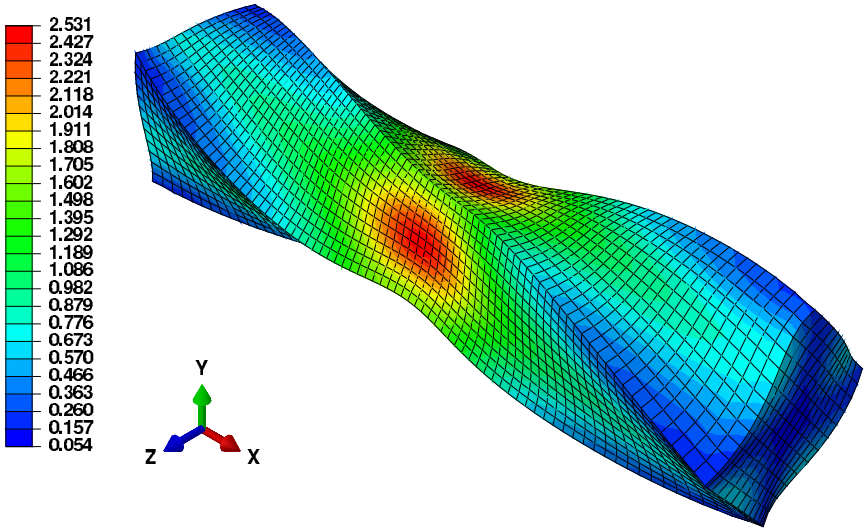
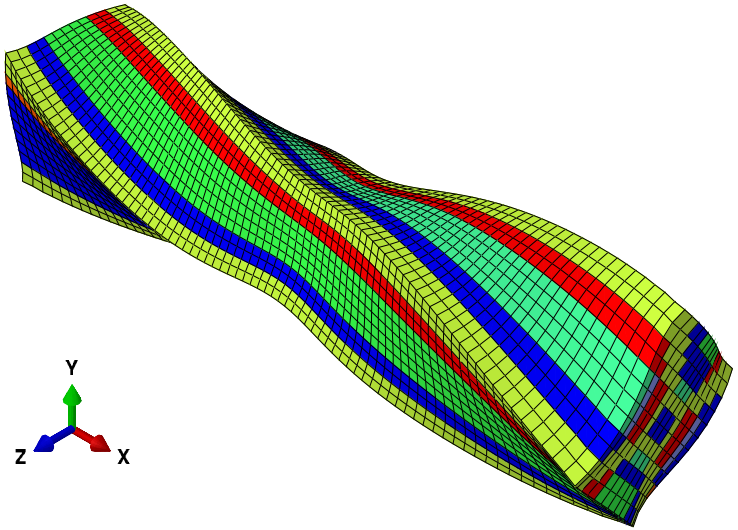




- Static clustering does not follow the evolution of the control field variable.
- Not much can be gained by simply increasing the number of clusters – an adaptive approach is needed.

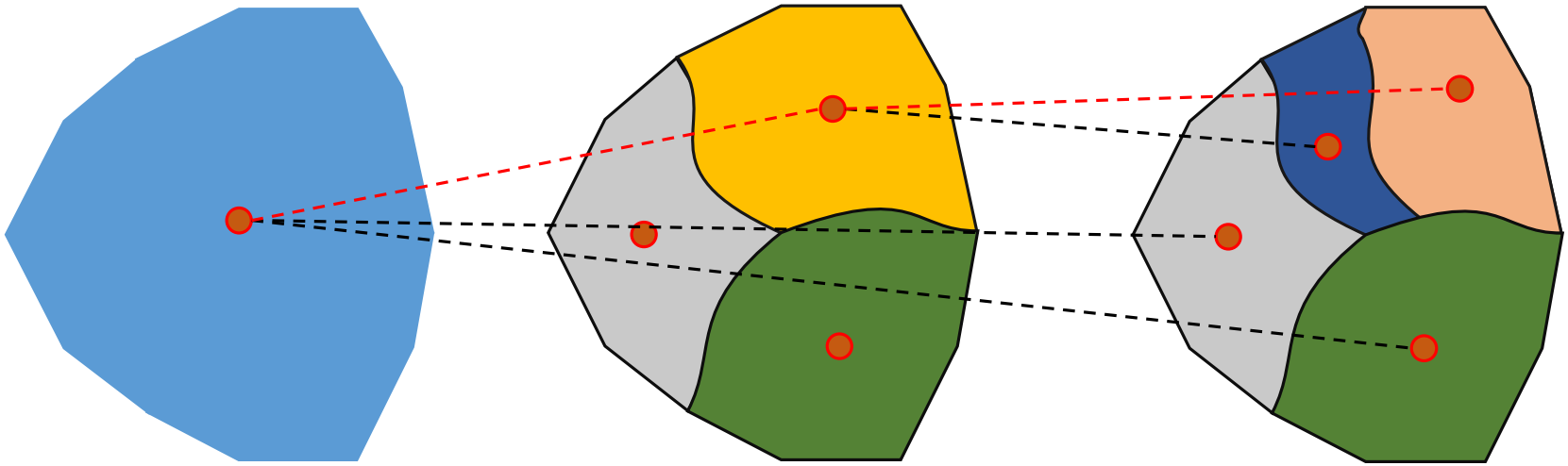
Dynamic adaptive clustering

- Parameter: threshold value t_{split}.
- Initialization: all points belong to a single cluster
- At each updating event, consider splitting each existing cluster C:

  1. $\Delta_{max} v = \max_{i \in C}(v_i) - \min_{i \in C}(v_i)$, where v is the control field variable.
  2. If $\Delta_{max} v \geq t_{split}$, re-cluster C into new clusters $C_1, \ldots, C_n$ that inherit the extended material states from the representative of C to the new representatives of $C_1, \ldots, C_n$.

- A high threshold value permits the clusters to persist longer; fewer clusters are generated overall, resulting in a high speedup but lower accuracy.

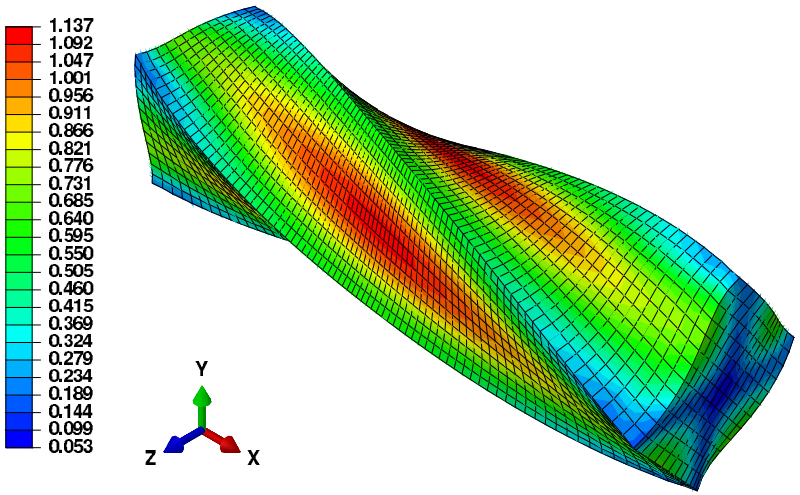
Dynamic clustering: the "split" operation

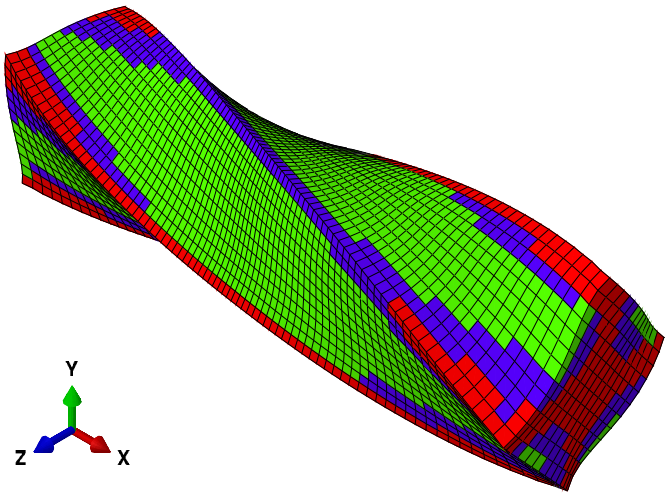


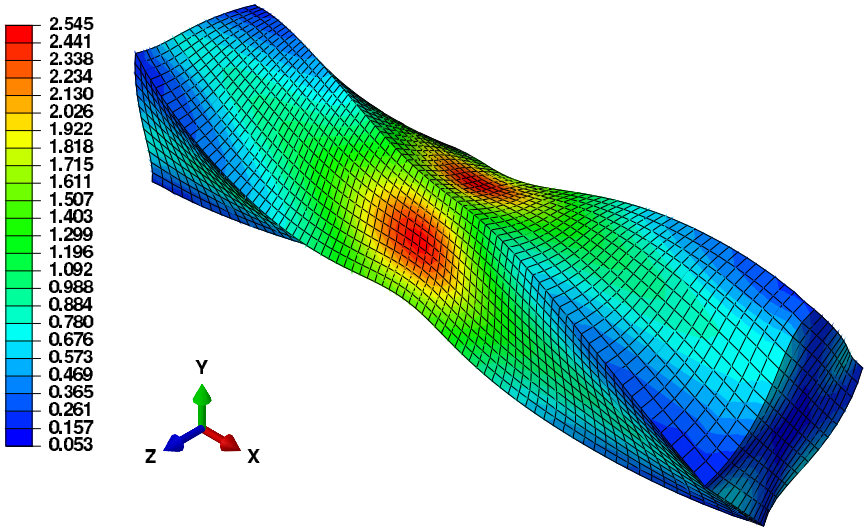
- Local operation on a limited number of integration points
  - think of divisive hierarchical clustering: $O(N^2)$, or DBSCAN or OPTICS: $O(n \log n)$)
- Direct back-traceability of the fine-scale model state variables

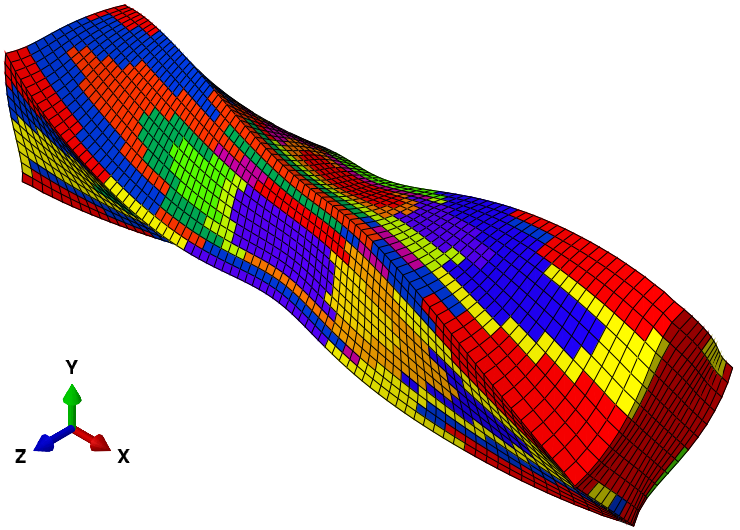
Dynamic adaptive clustering: results

Example: torque bar, high threshold for splitting









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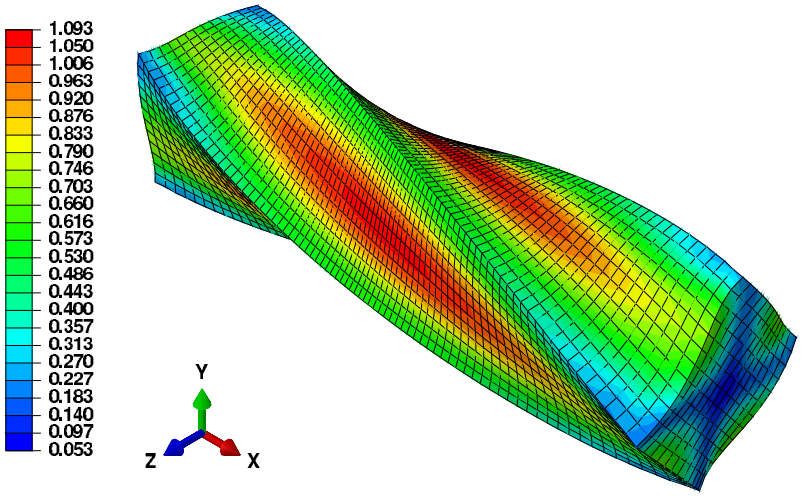
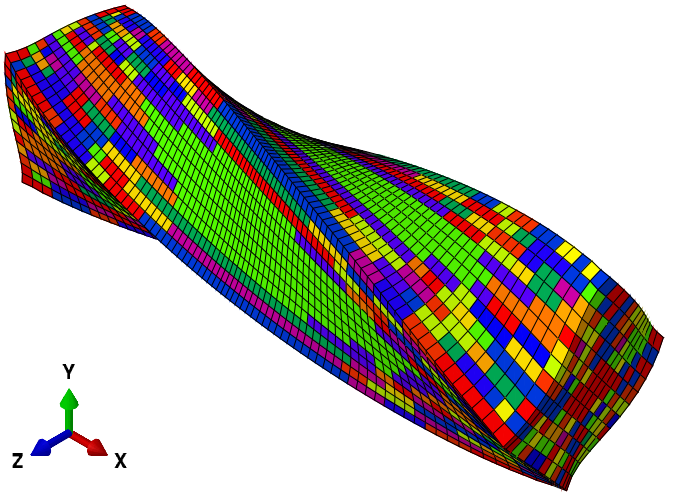
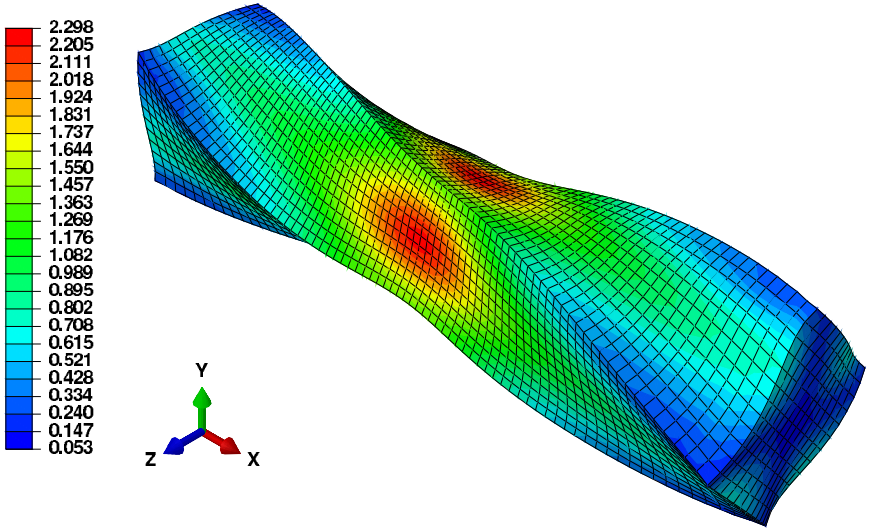
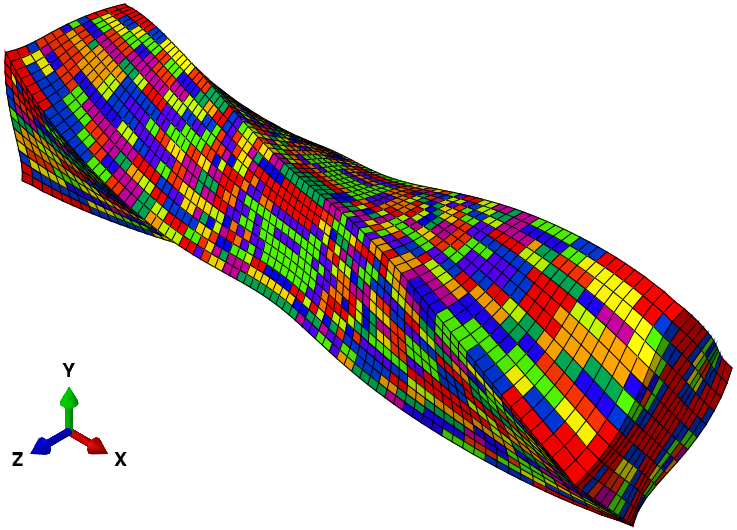
Dynamic adaptive clustering: results

Example: torque bar, low threshold for splitting









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Approximation error: material properties

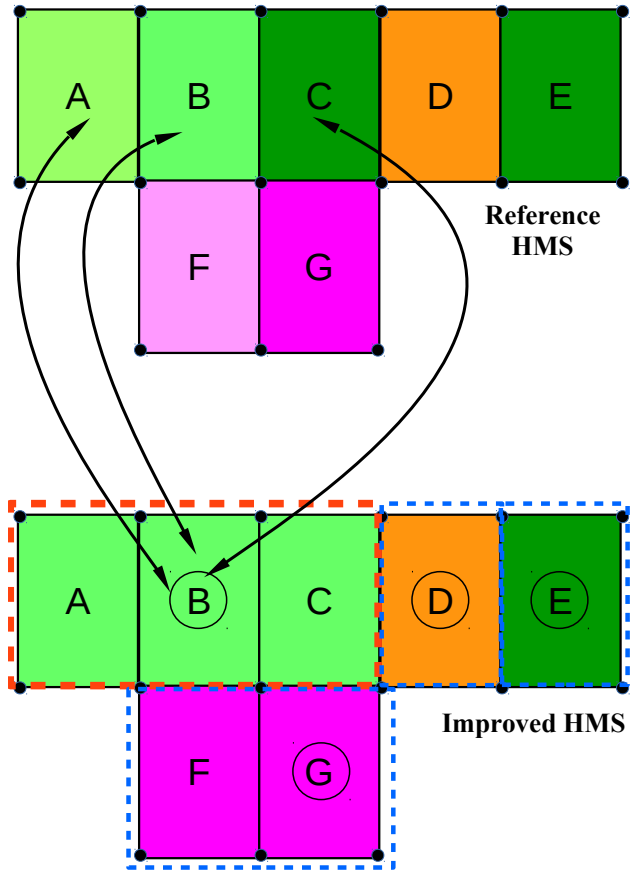
Reference HMS vs. clustering-enabled HMS

In terms of plastic potential function ψ, the relative error at integration point i:

$$e_i^{\psi} = \frac{1}{m} \sum_{j=1}^{m} \left| \frac{\psi(\mathbf{D}_j)_i - \psi'(\mathbf{D}_j)_{cr(i)}}{\psi(\mathbf{D}_j)_i} \right| \times 100\%$$

Error for the whole model:

$$\bar{e^{\psi}} = \frac{1}{n} \sum_{i=1}^{n} e_i^{\psi},$$



Approximation error: field variables

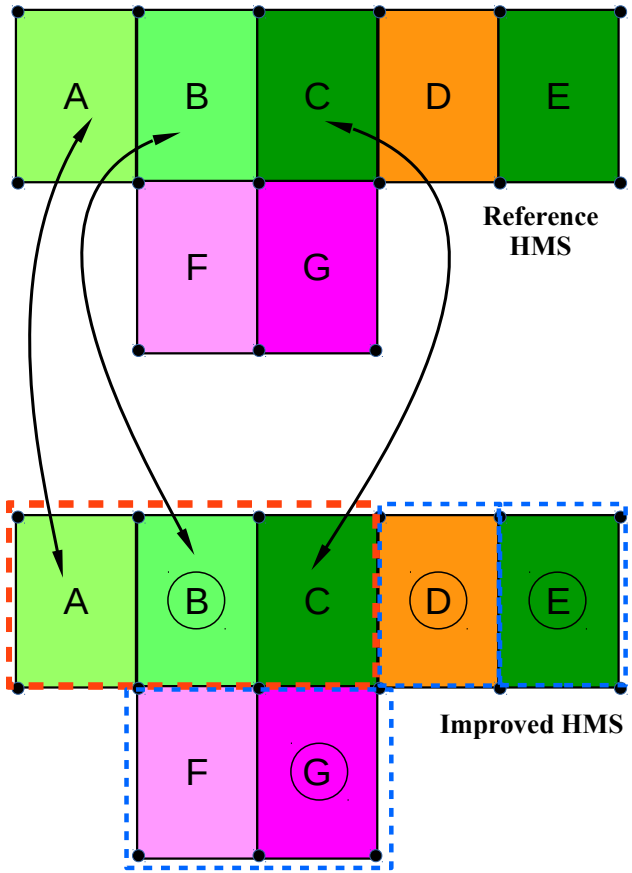
Reference HMS vs. clustering-enabled HMS

With respect to the field variable γ, the relative error at integration point i:

$$e_i^{\gamma} = \frac{|\gamma_i - \gamma_i'|}{\gamma_i} \times 100\%$$

Error for the whole model:

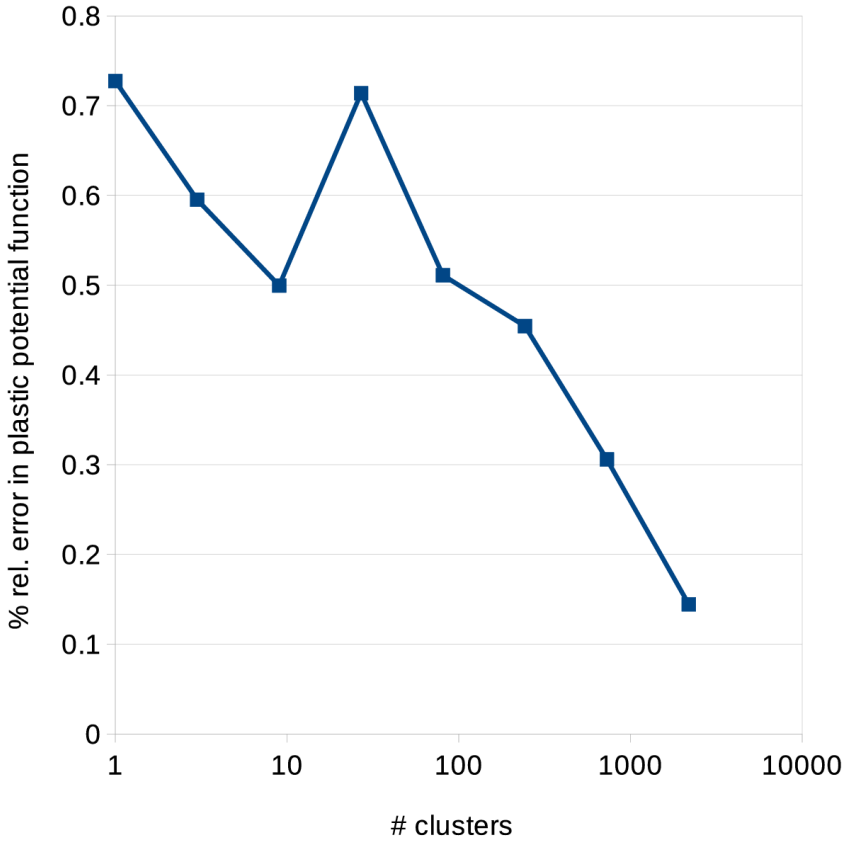
$$\bar{e^{\gamma}} = \frac{1}{n} \sum_{i=1}^{n} e_i^{\gamma}$$



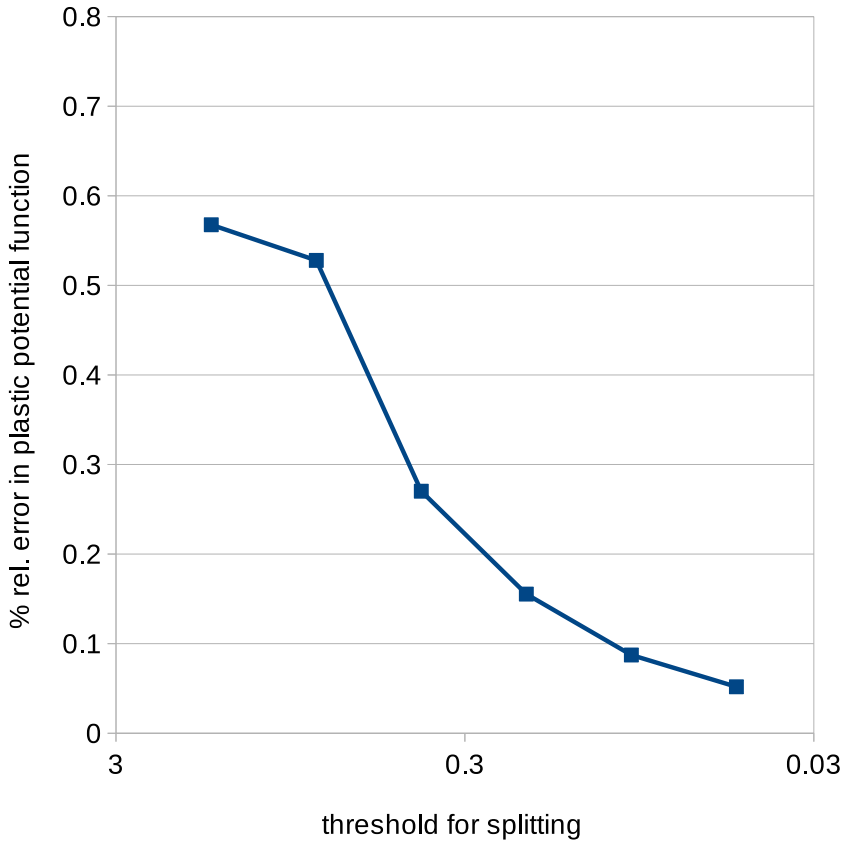
Note: γ is the control variable used in clustering.

Accuracy of static and dynamic clustering schemes

Material property: plastic potential



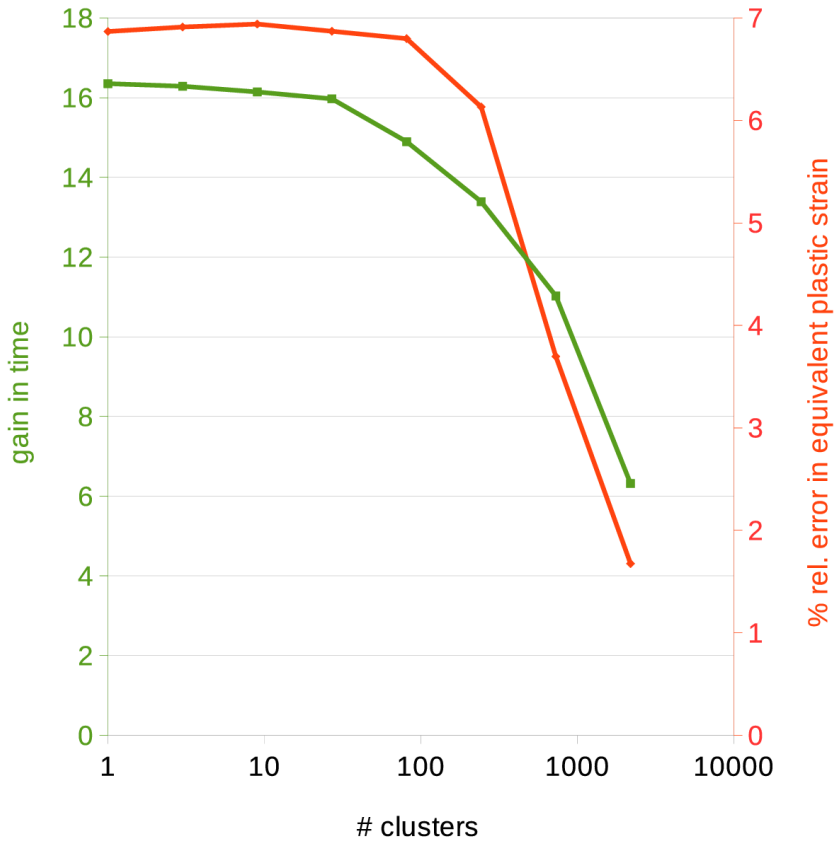
static clustering scheme



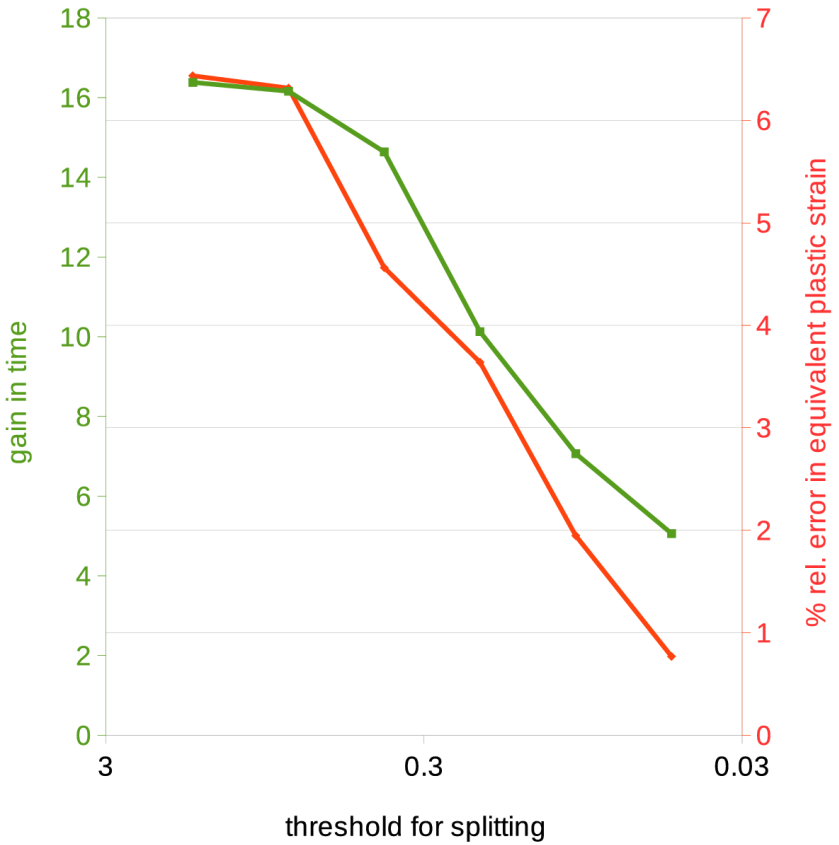
dynamic clustering scheme

Accuracy of static and dynamic clustering schemes

Plastic strain

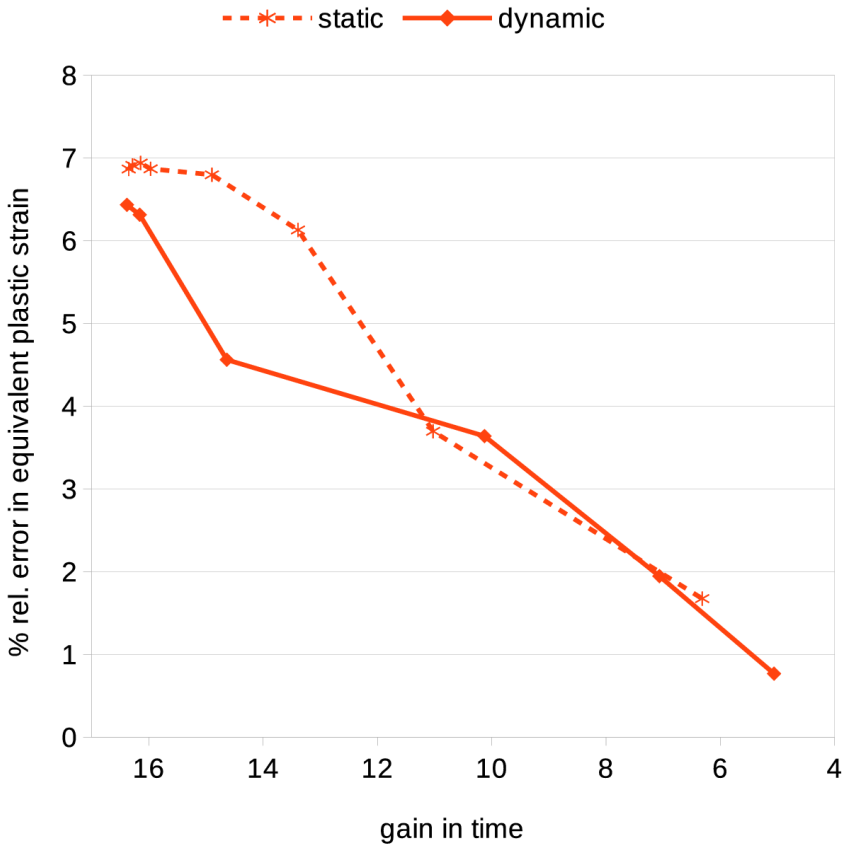


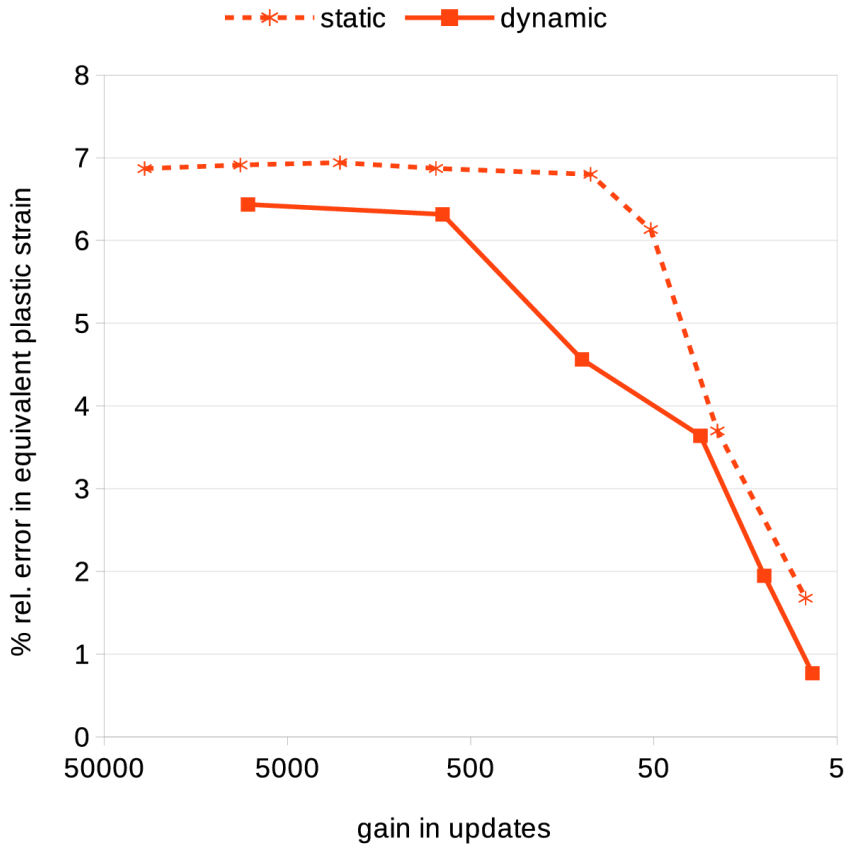
static clustering scheme



dynamic clustering scheme

Performance gain: static vs. dynamic clustering scheme





Overall gain in total computation time (speedup):

$$g_t = \frac{t_r}{t_c}$$

Reduction in the number of calls to the fine-scale model ("speedup in updates"):

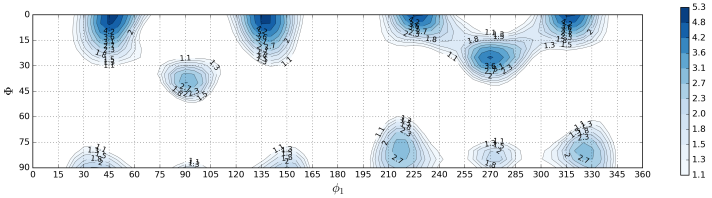
$$g_u = \frac{n_r}{n_c}$$

Microstructural similarity within clusters

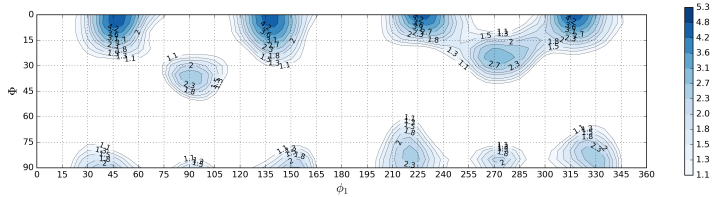
Example: dynamic clustering scheme, torque bar

Recall the assumption we made:

similar deformation in adjacent points $\Rightarrow$ similar microstructures $\Rightarrow$ similar properties



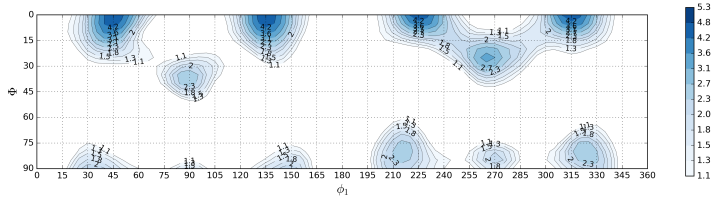
cluster representative point (RP)

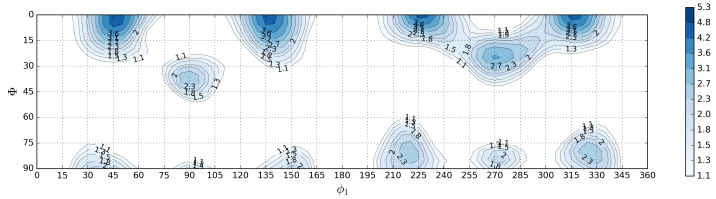


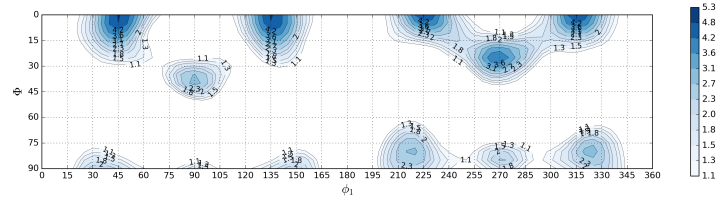
corresponding point in the reference HMS

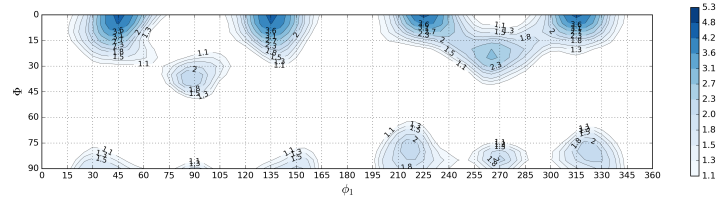
Do actually similar microstructures develop if neighboring points are subjected to similar deformation?

$\rightarrow$ Yes, see deformation textures at several points of the reference HMS that would belong to the same cluster:









Summary and take-aways

1. The HMS adaptively approximates mechanical responses of the CP model by much simpler analytical models.
2. Concurrent evolution of texture and plastic anisotropy can be then handled in component-scale FE models.
3. Further acceleration of the HMS is attained if spatial quasi-homogeneities are exploited.
4. Static and dynamic clustering schemes restrict tracking the evolution of the fine-scale variables to a number of representative material points.
5. Large performance gains (e.g. a speedup of 25) are attained at the expense of minor modelling error.
6. Dynamic clustering scheme in the HMS allows following the field of interest.

Advanced solutions for component-scale crystal plasticity simulations by KU Leuven Knowledge Platform M2Form:

HMS : Hierarchical Multi-Scale framework

VEF : Virtual Experimentation Framework

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