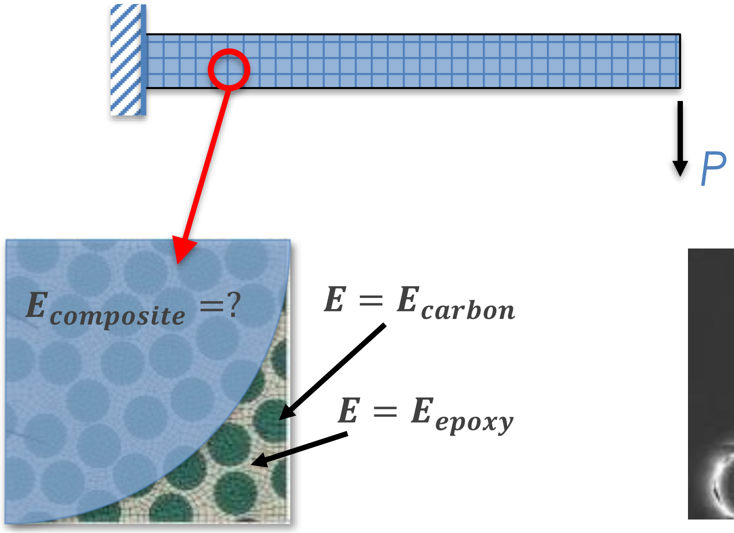
Direct FE^2 – Concurrent multiscale modelling with commercial finite element codes

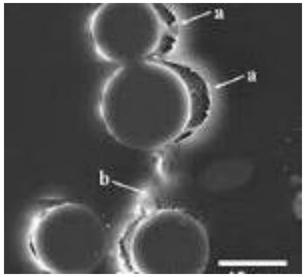
K Raju, J Zhi, LH Poh, TE Tay, *Vincent BC Tan*

Introduction

What is FE[2] ?

- A two-scale finite element analysis of structures of heterogeneous materials.
- Traditionally implemented when
  - the constitutive property of heterogenous material is unavailable, or
  - microstructural changes during loading affect constitutive property
- Comprises macroscale FEA of structure with many microscale FEA of unit cells/RVEs to obtain homogenized properties





Fibre debond

Single scale FEA

Static stress analysis

$$\sigma_{ij,j} + b_i = 0$$

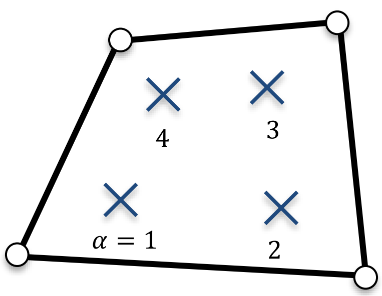
$$\Rightarrow \underbrace{\int_V \delta\varepsilon_{ij}\sigma_{ij}\,dV}_{\delta W_{int}} = \underbrace{f_I \delta u_I}_{\delta W_{ext}}$$

Numerical integration

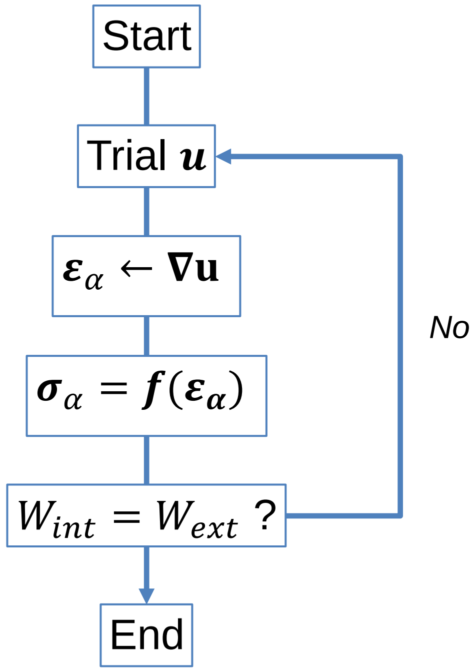
$$\Rightarrow \delta W_{int} = \sum_{\alpha} w_\alpha J_\alpha \left(\delta\varepsilon_{ij}\right)_\alpha \left(\sigma_{ij}\right)_\alpha$$

Gaussian weight

Jacobian determinant $|J_\alpha|$



4-node quad element with 2x2 gauss points



Multiscale FEA with FE^2

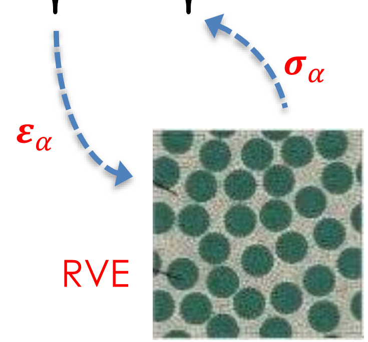
Static stress analysis

$$\sigma_{ij,j} + b_i = 0$$

$$\Rightarrow \int_V \underbrace{\delta\varepsilon_{ij}\sigma_{ij}\, dV}_{\delta W_{int}} = \underbrace{f_I \delta u_I}_{\delta W_{ext}}$$

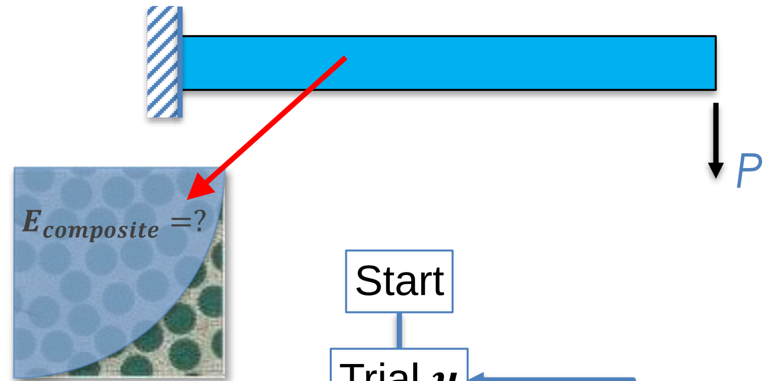
Numerical integration

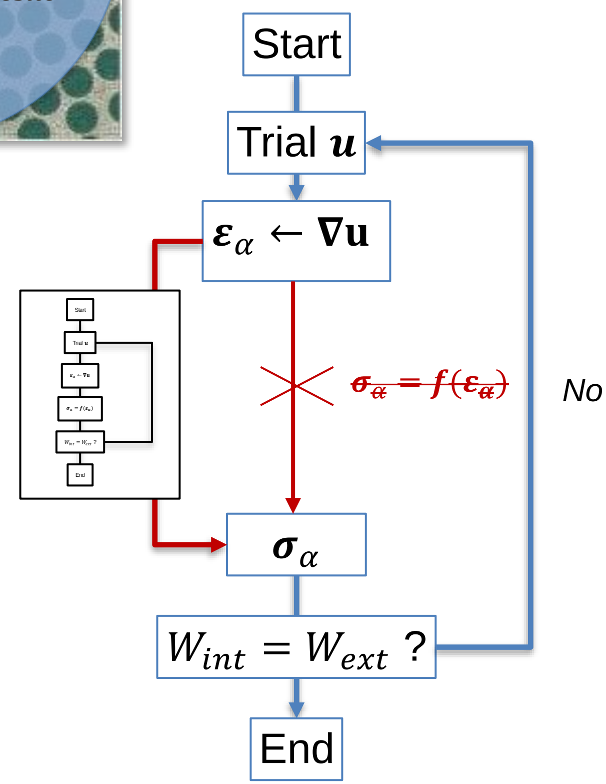
$$\Rightarrow \delta W_{int} = \sum_{\alpha} w_\alpha J_\alpha \underbrace{\left(\delta\varepsilon_{ij}\right)_\alpha}_{} \underbrace{\left(\sigma_{ij}\right)_\alpha}_{}$$



Microscale FEA

Macroscale FEA

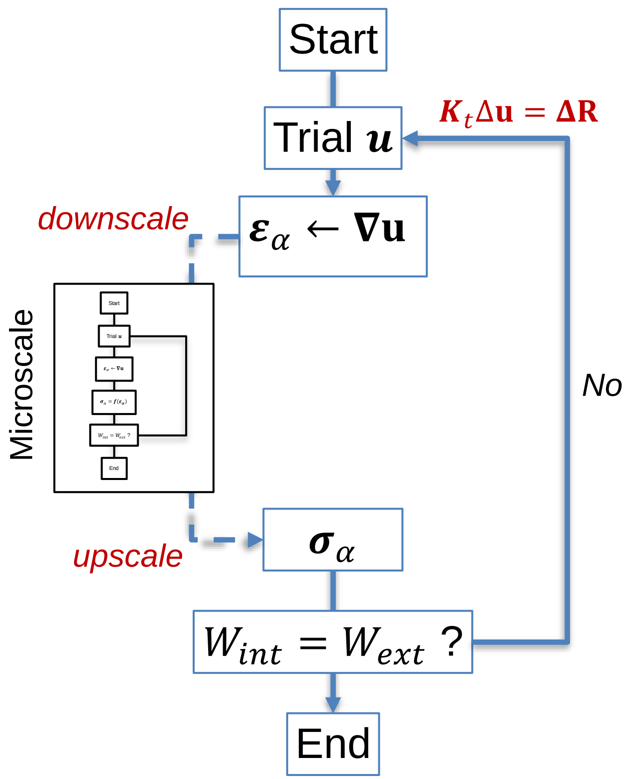


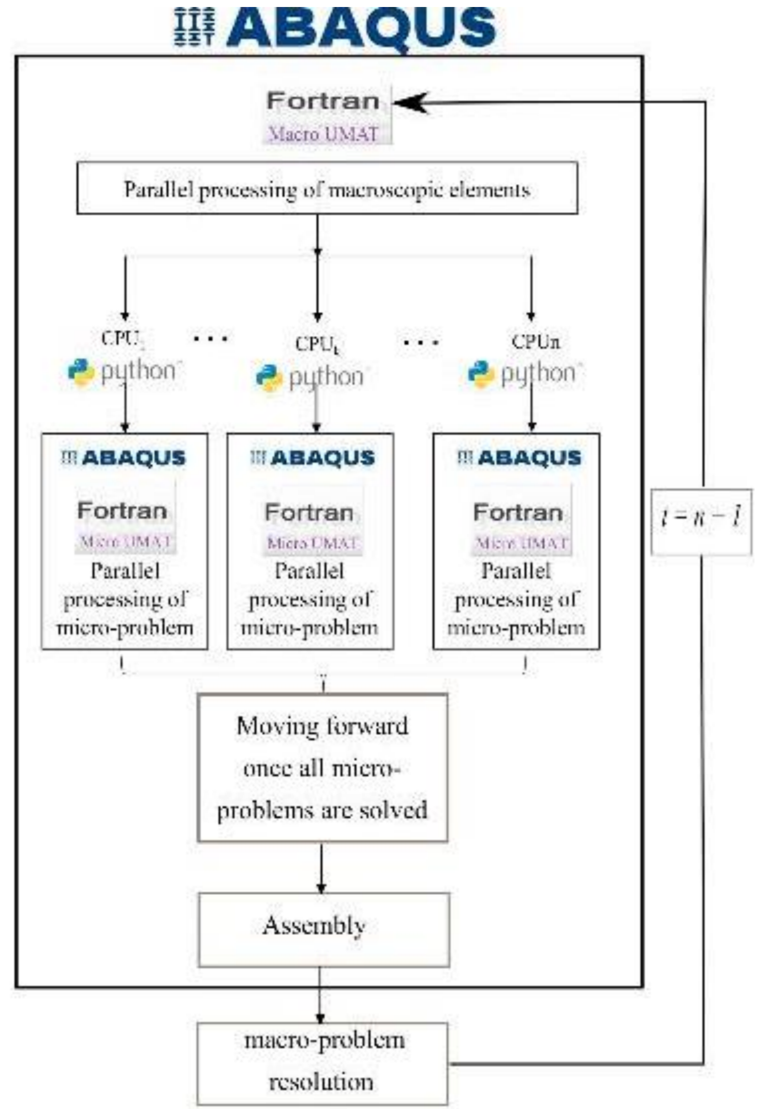


Conventional FE^2

Typical implementation

- Separate FE jobs for macroscale and RVEs
- Codes for downscaling and upscaling information exchange
- User defined material routine at macroscale including tangent stiffness, K_t



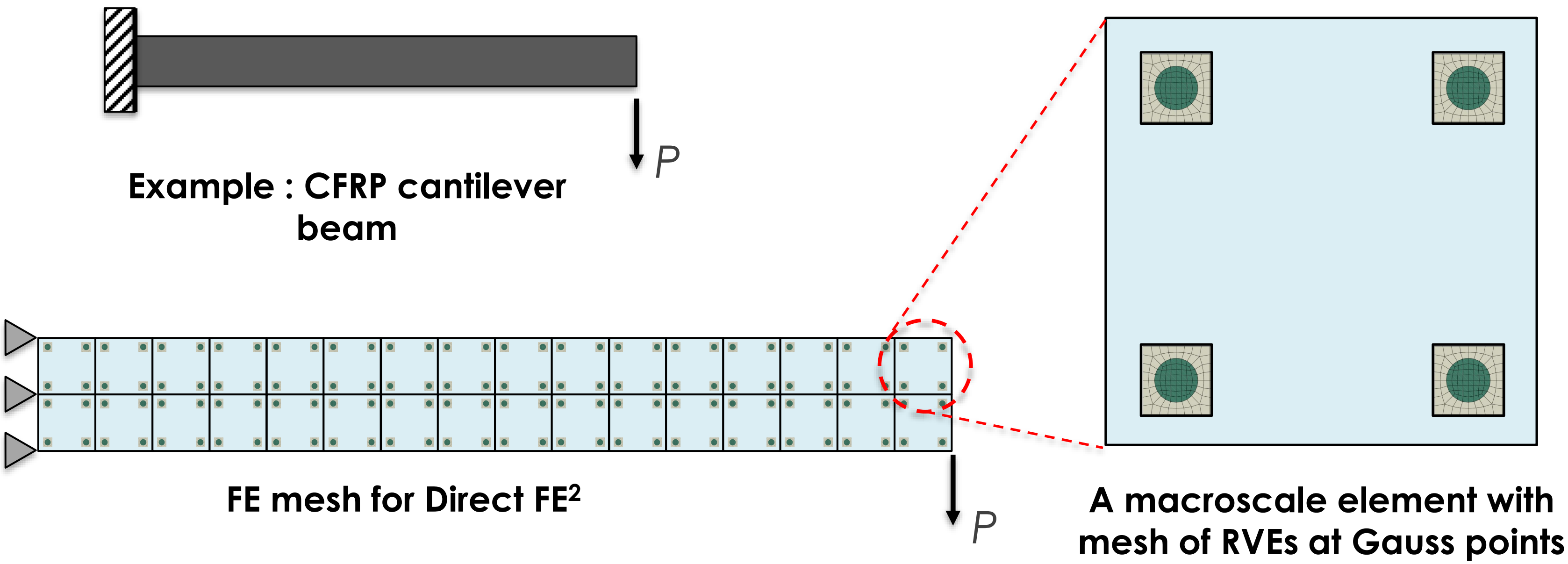


Composite Structures, 193, (2018)

Setting up Direct FE²

1. Combined dual scale mesh

In Direct FE², 2 levels of finite elements appear together as a single FE mesh



- The CFRP beam is meshed with 2×16 macro elements. Each macro-element has the mesh of 4 RVEs at its Gauss points.
- Macro elements and RVE elements appear together as a single ABAQUS mesh and run as a single job.

Setting up Direct FE^2

2. Kinematic constraints

Constraints are applied so that the RVEs deform with the macro-scale elements.

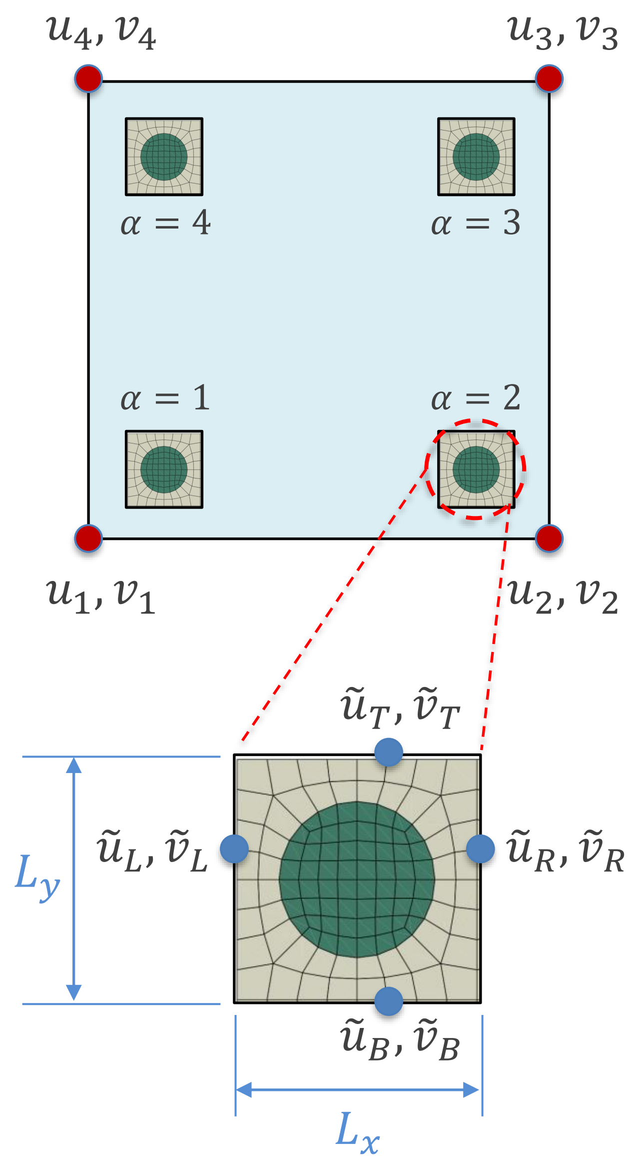
At the macroscale, the deformation gradients are,

$$\begin{matrix} u = \sum N_I u_I \\ v = \sum N_I v_I \end{matrix} \Rightarrow \begin{matrix} u_{,x} = \sum N_{I,x} u_I \\ v_{,x} = \sum N_{I,x} v_I \end{matrix}, \quad \begin{matrix} u_{,y} = \sum N_{I,y} u_I \\ v_{,y} = \sum N_{I,y} v_I \end{matrix}$$

These are applied as Periodic Boundary Conditions to the RVEs

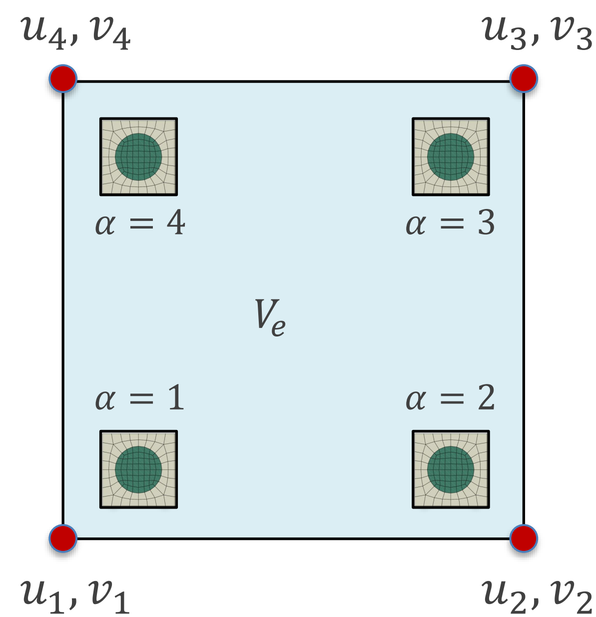
$$\begin{matrix} \dfrac{\tilde{u}_R - \tilde{u}_L}{L_x} = \sum N_{I,x} u_I \\ \dfrac{\tilde{v}_R - \tilde{v}_L}{L_x} = \sum N_{I,x} v_I \end{matrix}, \quad \begin{matrix} \dfrac{\tilde{u}_T - \tilde{u}_B}{L_y} = \sum N_{I,y} u_I \\ \dfrac{\tilde{v}_T - \tilde{v}_B}{L_y} = \sum N_{I,y} v_I \end{matrix}$$

The above relations between the RVE and macroscale nodes are applied only once using MPC (multipoint constraints) in ABAQUS at the pre-processing stage.



Setting up Direct FE^2

3. Energy consistency



Strain energy within each macroscale element is calculated using Gaussian quadrature,

$$\delta W_{int} = \int_{V_e} \delta \boldsymbol{\varepsilon} : \boldsymbol{\sigma} \, dV = \sum_{\alpha} w_\alpha J_\alpha \delta \boldsymbol{\varepsilon}_\alpha : \boldsymbol{\sigma}_\alpha$$

In a FE^2 analysis, $\boldsymbol{\sigma}_\alpha$ cannot be directly determined because the constitutive relation at the macroscale is unknown.

Instead, $\delta \boldsymbol{\varepsilon}_\alpha : \boldsymbol{\sigma}_\alpha$ is replaced by the average energy densities of the RVEs

$$\delta \boldsymbol{\varepsilon}_\alpha : \boldsymbol{\sigma}_\alpha \equiv \frac{1}{V_\alpha} \int_{V_\alpha} \delta \tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$ ← *Hill-Mandel condition*

$$\Rightarrow \delta W_{int} = \sum_{\alpha} \frac{w_\alpha J_\alpha}{V_\alpha} \int_{V_\alpha} \delta \tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$

Setting up Direct FE^2

3. Energy consistency

In Direct FE^2, the macroscale element is assigned zero material properties.

Therefore, internal energy calculated by ABAQUS is from the RVEs only, i.e.,

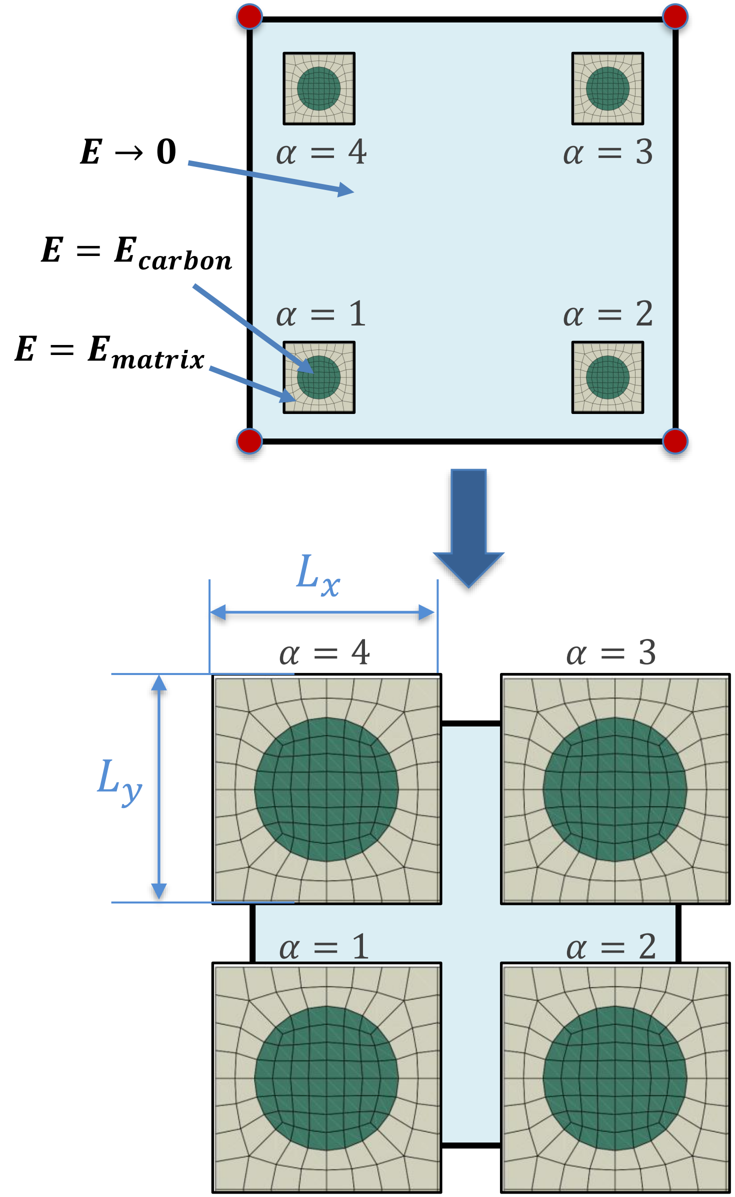
$$\delta W_{int}^{FE^2} = \sum_{\alpha} \int_{V_\alpha} \delta\tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$

To obtain the correct internal energy, we must make $\delta W_{int}^{FE^2}$ equal to

$$\delta W_{int} = \sum_{\alpha} \frac{w_\alpha J_\alpha}{V_\alpha} \int_{V_\alpha} \delta\tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$

Hence, we choose the dimensions of the RVE, i.e., L_x and L_y, so that

$$V_\alpha = w_\alpha J_\alpha$$



Setting up Direct FE^2

3. Energy consistency

In Direct FE^2, the macroscale element is assigned zero material properties.

Therefore, internal energy calculated by ABAQUS is from the RVEs only, i.e.,

$$\delta W_{int}^{FE^2} = \sum_{\alpha} \int_{V_\alpha} \delta\tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$

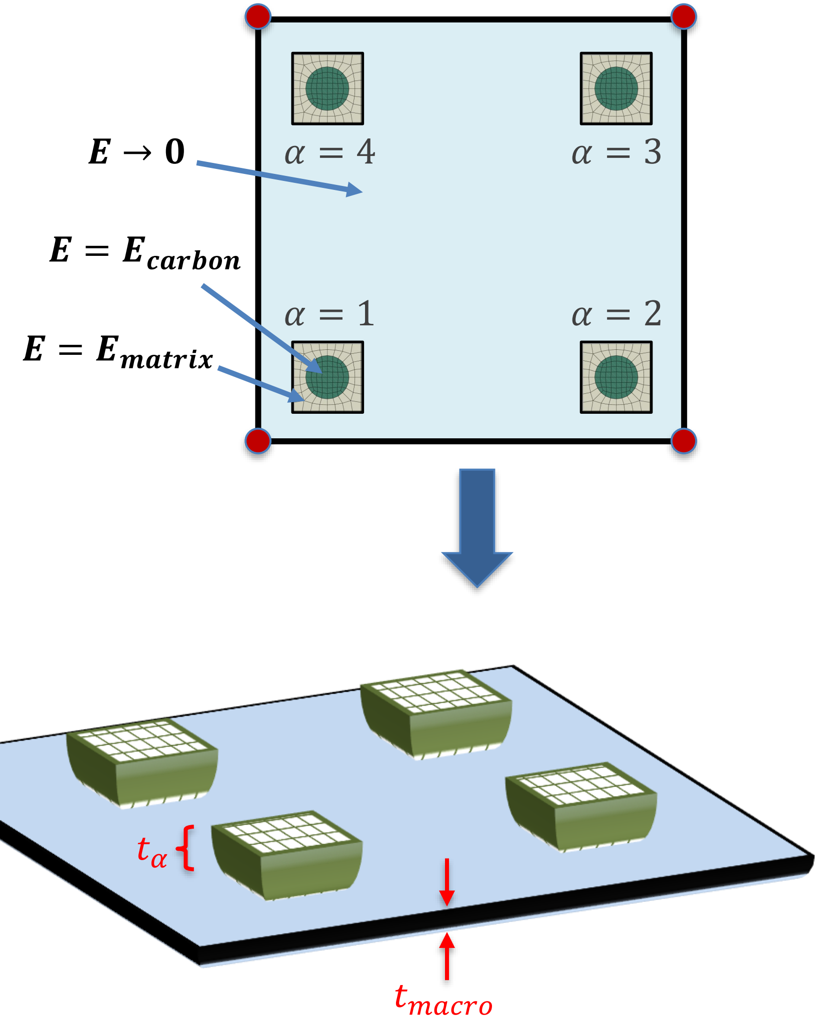
To obtain the correct internal energy, we must make $\delta W_{int}^{FE^2}$ equal to

$$\delta W_{int} = \sum_{\alpha} \frac{w_\alpha J_\alpha}{V_\alpha} \int_{V_\alpha} \delta\tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\sigma}} \, dV$$

Hence, we choose the dimensions of the RVE, i.e., L_x and L_y, so that

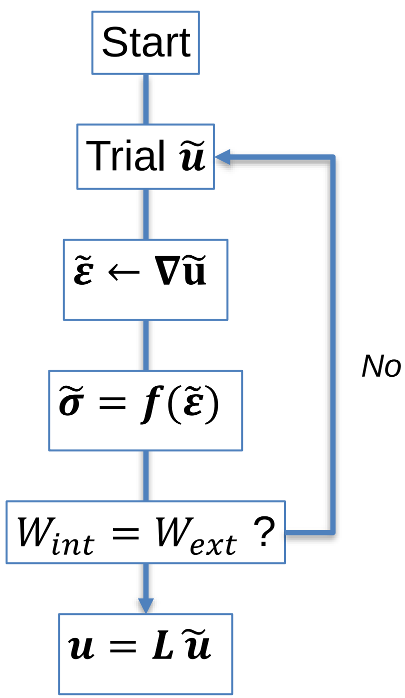
$$V_\alpha = w_\alpha J_\alpha$$

For 2D analysis, the thickness can be scaled instead.



Direct FE^2 vs conventional FE^2

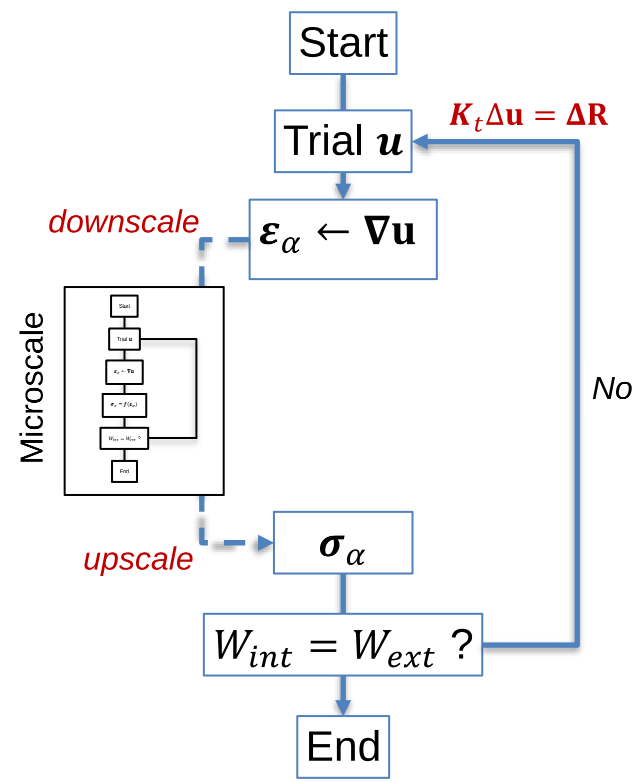
Direct FE^2



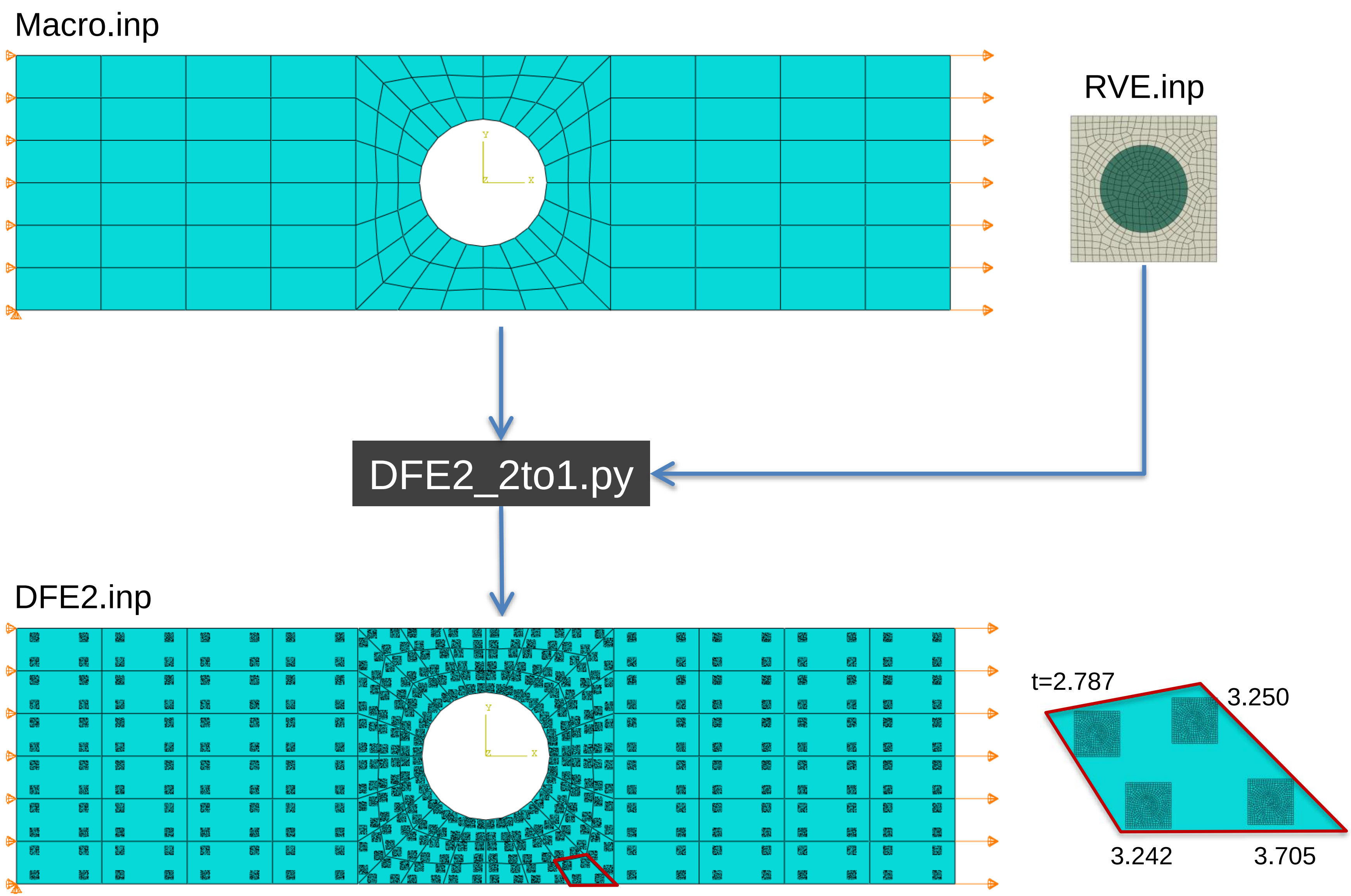
Steps :

- Determine scaled volume of RVEs
- Set up macroscale and RVE mesh
- Apply MPC to establish kinematic constraints

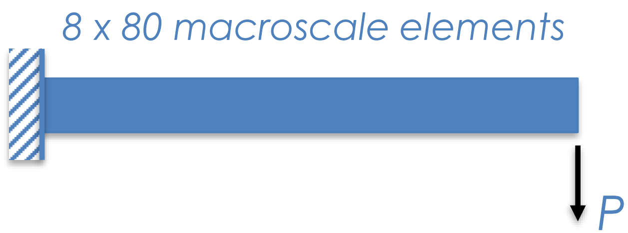
Conventional FE^2



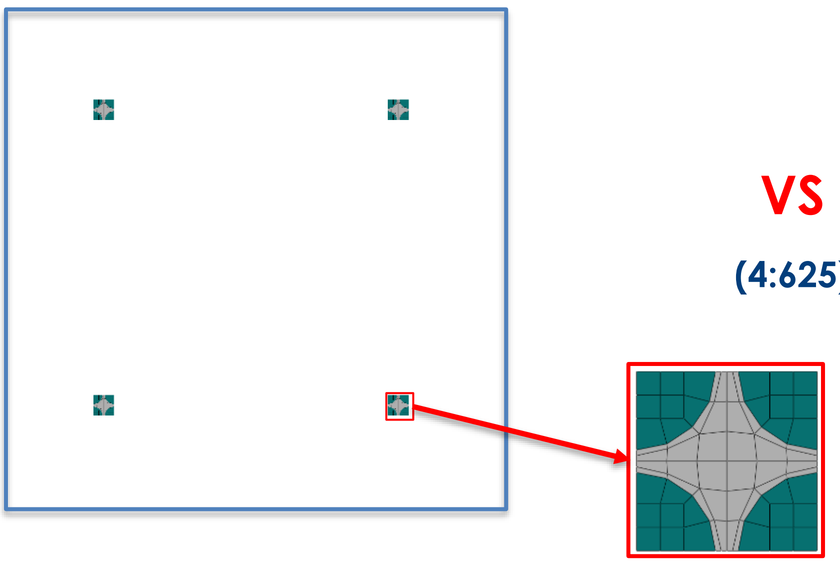
Python script for Direct FE^2



Direct FE^2 for composite beam



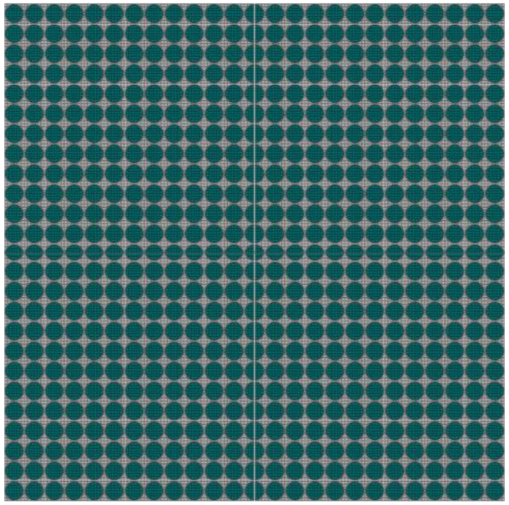
FE^2



VS

(4:625)

Full FE/DNS

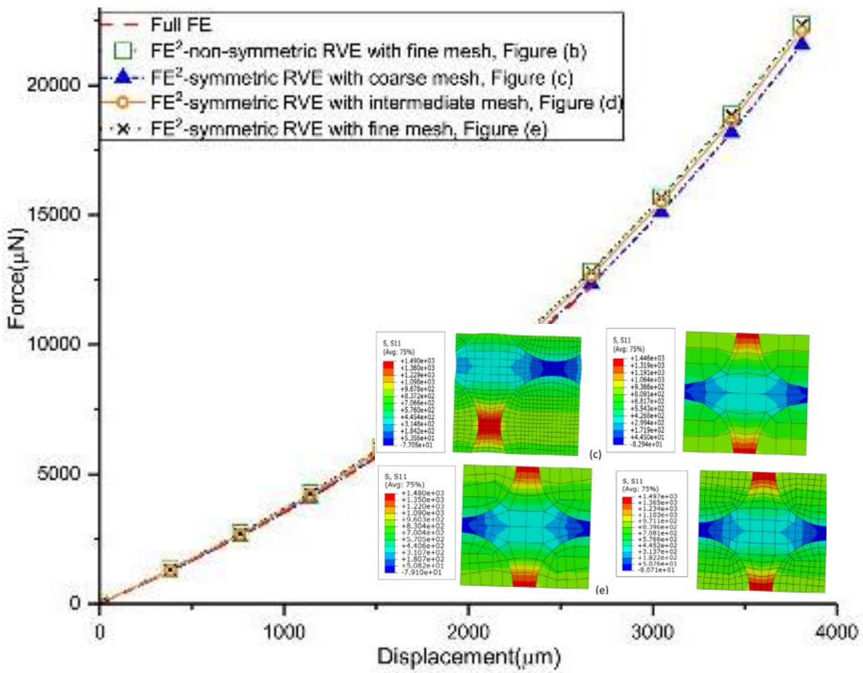


One macroscale element in FE^2 analysis

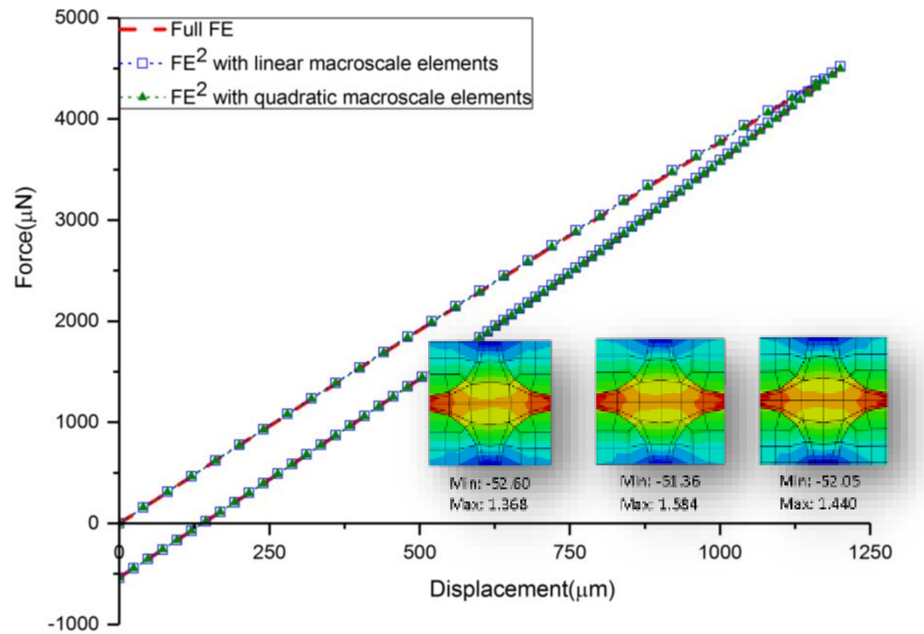
One macroscale element in full FE analysis

K. Raju, et al., Direct FE^2 for concurrent multilevel modelling of heterogeneous structures, (2020) CMAME, 360, 112694.

Direct FE^2 for composite beam



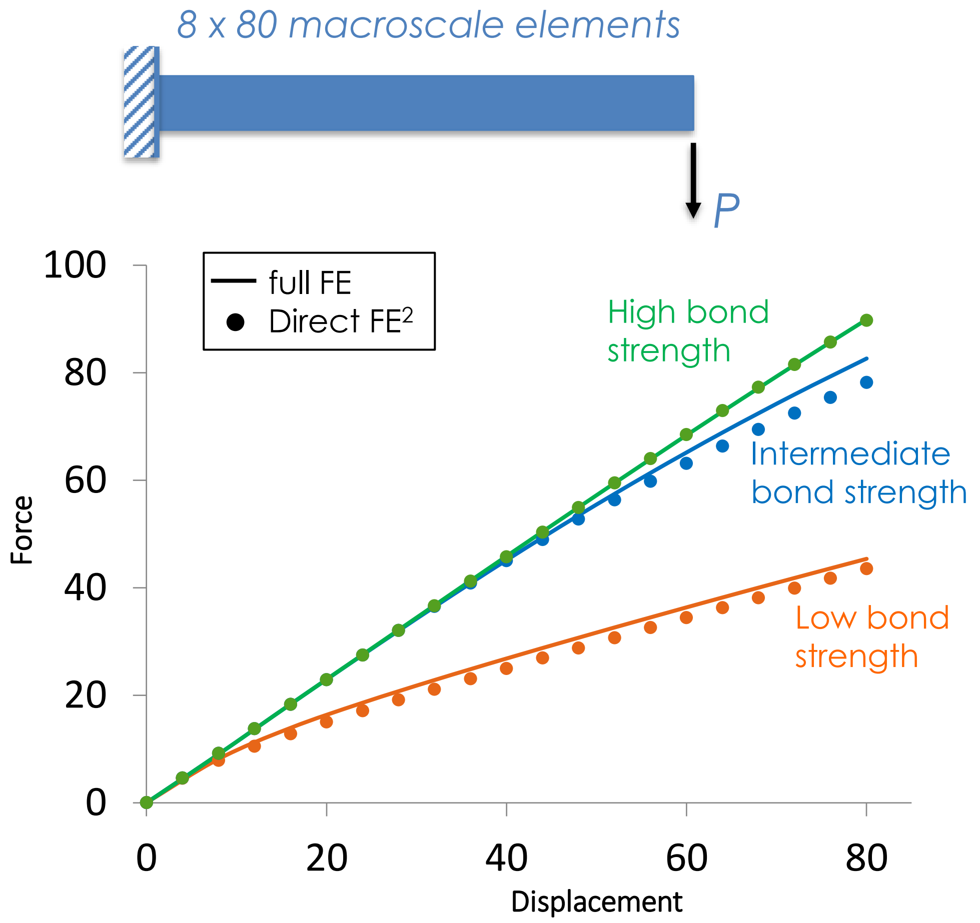
Load–displacement plots for large deformation elastic composite beam.

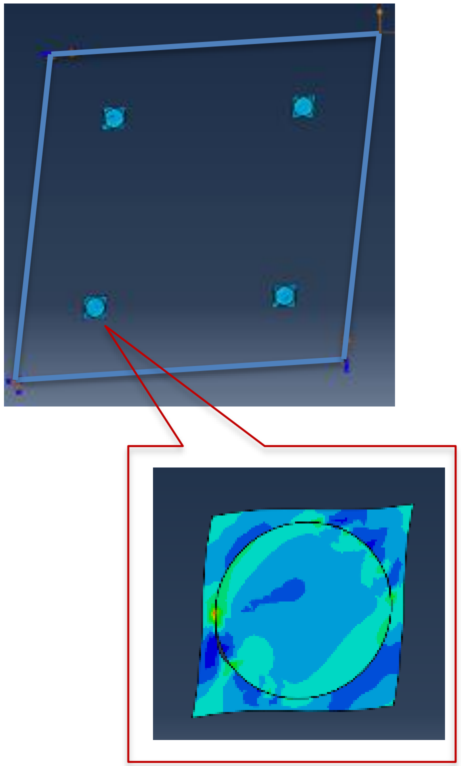


Load–displacement plots for viscoelastic composite beam.

K. Raju, et al., Direct FE^2 for concurrent multilevel modelling of heterogeneous structures, (2020) CMAME, 360, 112694.

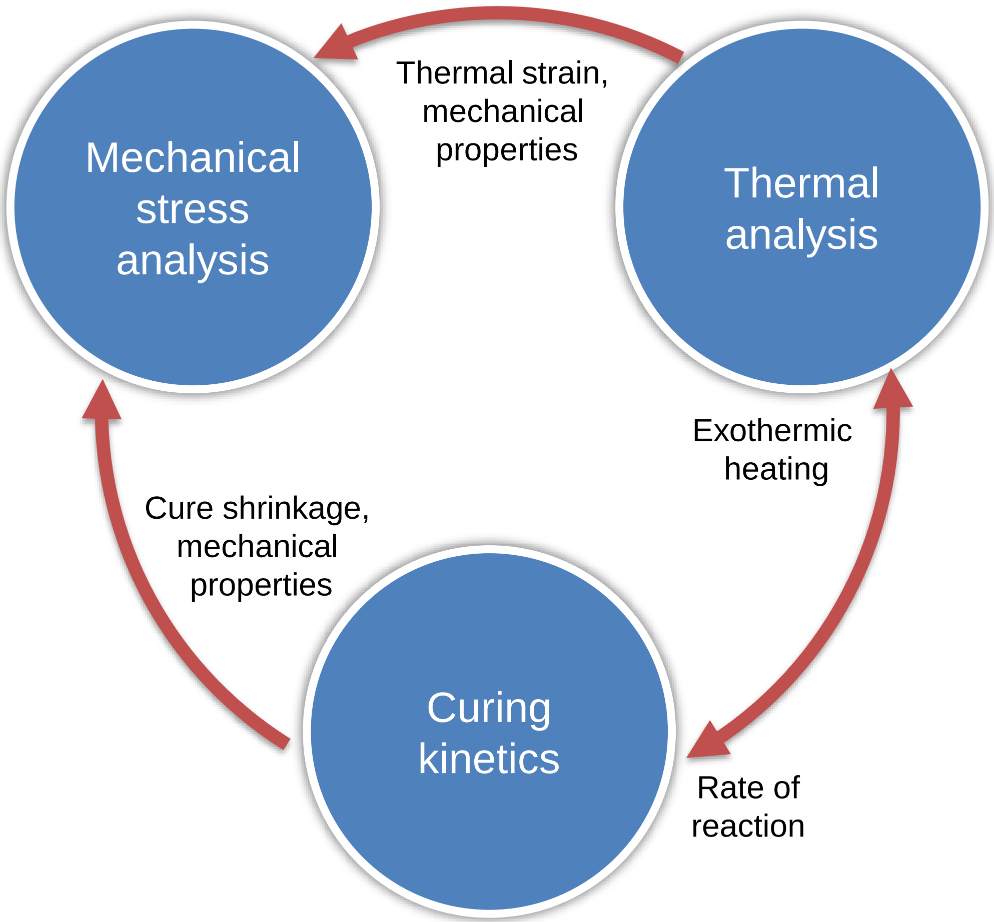
Direct FE^2 for composite beam





Load–displacement plots for composite beam with fibre debond.

Thermo-mechanical cure-induced deformation



<u>Interdependencies</u>:
(3501-6 epoxy)

- Modulus

$$E = E^{\infty} + (E^{u} - E^{\infty}) \sum_{n} w_n \exp\left(-\frac{\xi(\alpha, T)}{\zeta(\alpha)}\right)$$

- Exothermic heating

$$r = \rho H \dot{\alpha}$$

- Rate of cure

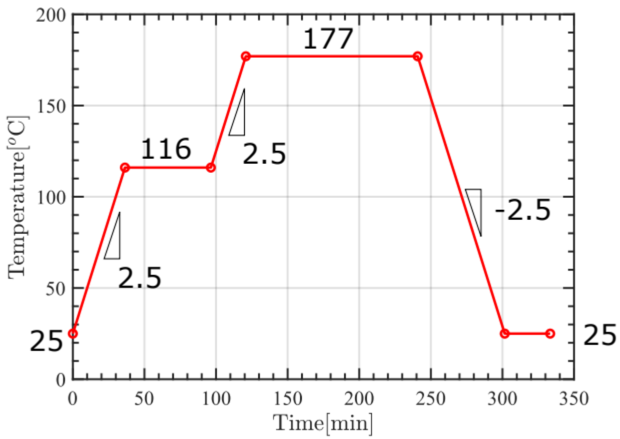
$$\dot{\alpha} = \begin{cases} (K_1 + K_2\alpha)(1-\alpha)(0.47-\alpha) & \alpha \le 0.3 \\ K_3(1-\alpha) & \alpha > 0.3 \end{cases}$$

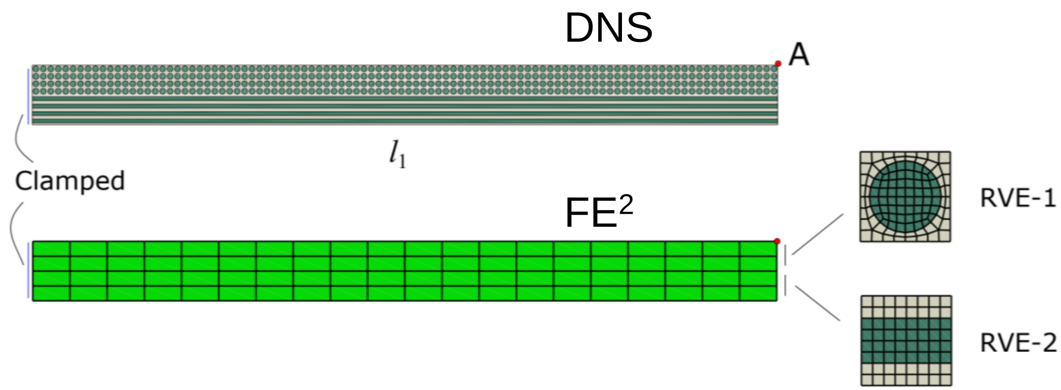
$$K_i = A_i \exp\left(-\frac{\Delta E_i}{RT}\right)$$

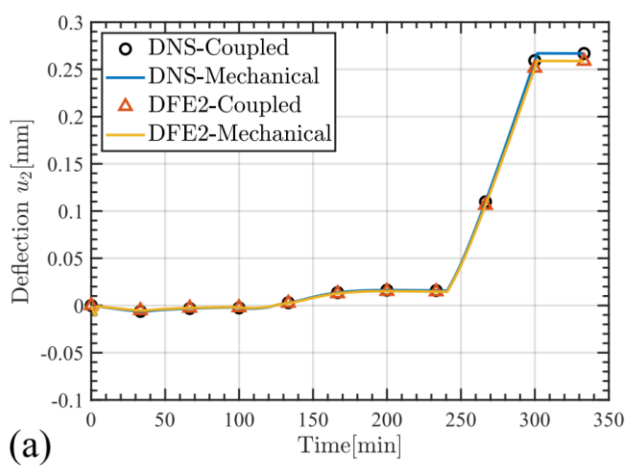
J Zhi, et al., Multiscale thermo-mechanical analysis of cure-induced deformation in composite laminates using Direct FE2, Composites Part A (2023), doi: https://doi.org/10.1016/j.compositesa.2023.107704..

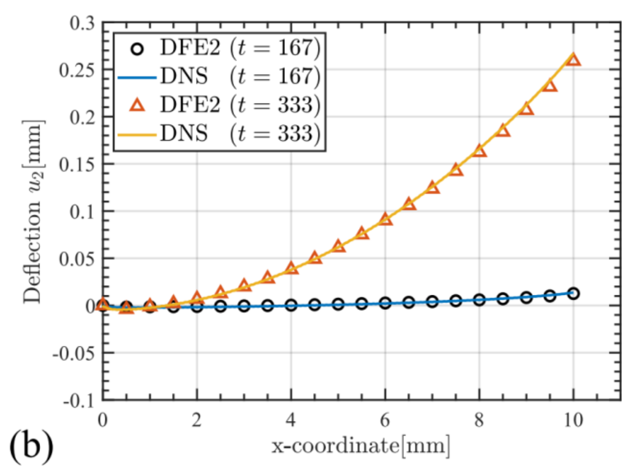
Thermo-mechanical cure-induced deformation

Cure cycle





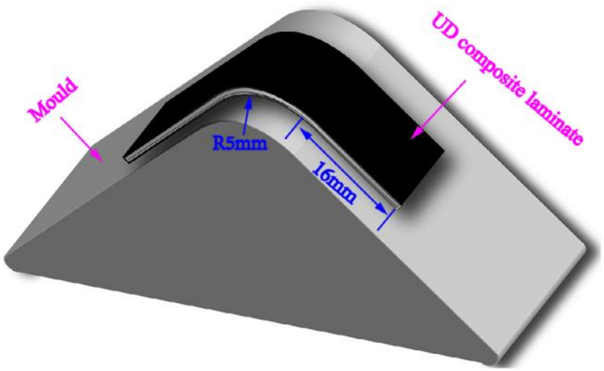


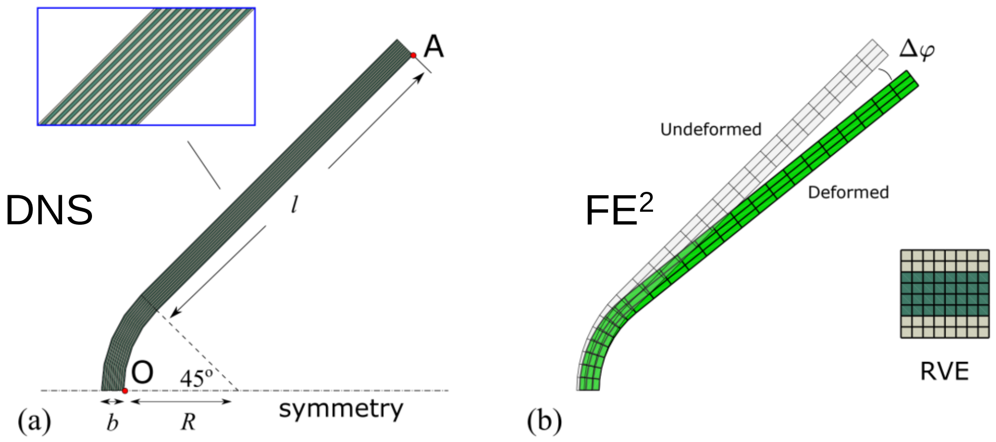


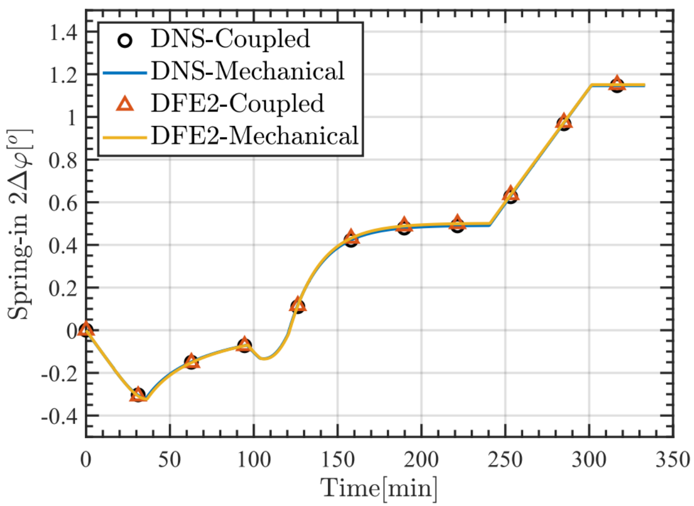
Deflection of point A vs time

Deflection of top edge

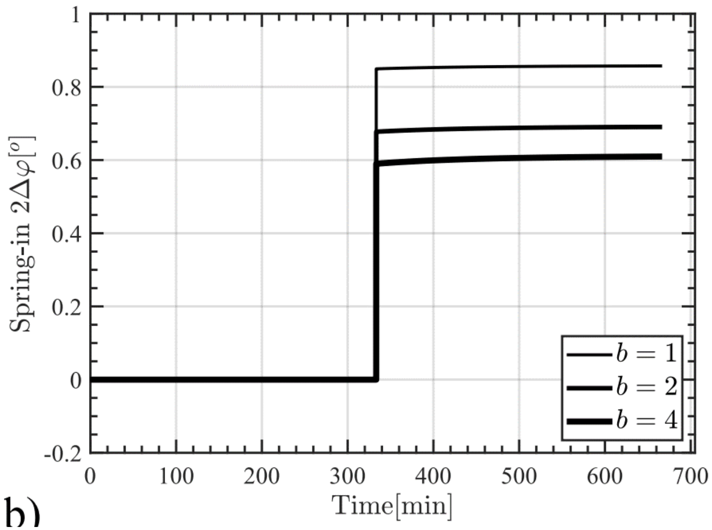
Thermo-mechanical cure-induced deformation





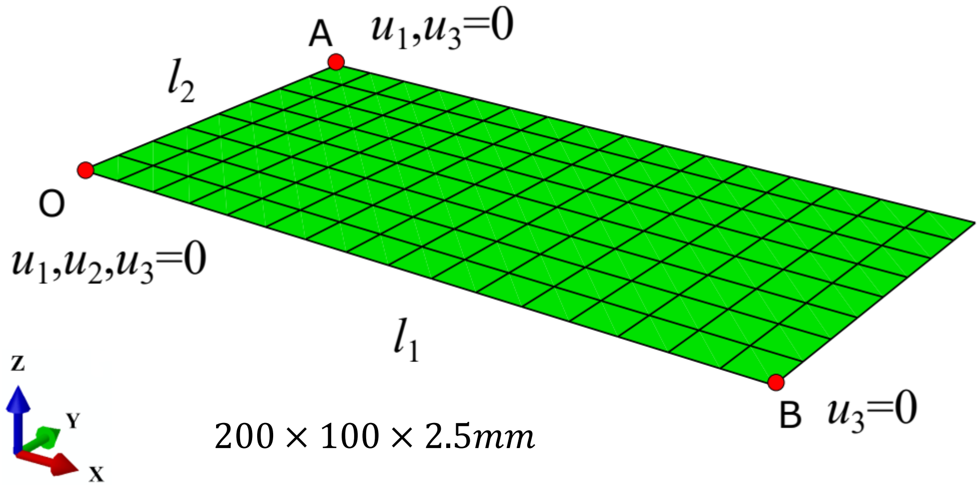


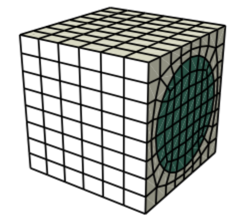
Spring-in vs time (unrestrained)



Spring-in vs time (restrained)

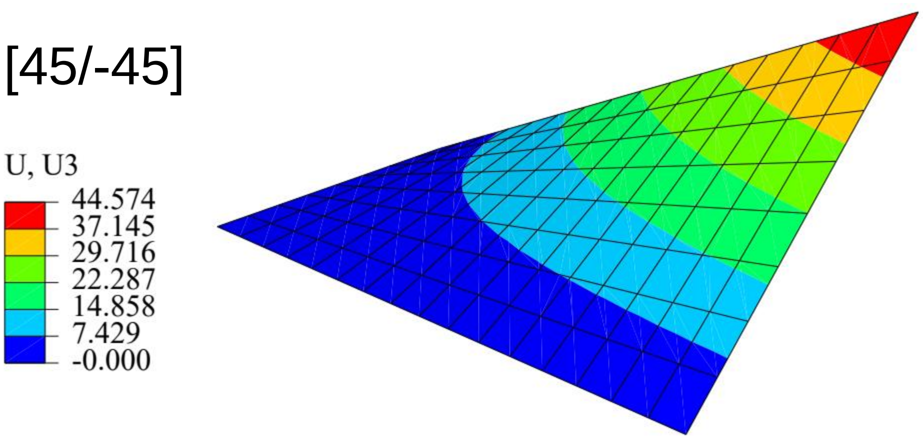
Thermo-mechanical cure-induced deformation

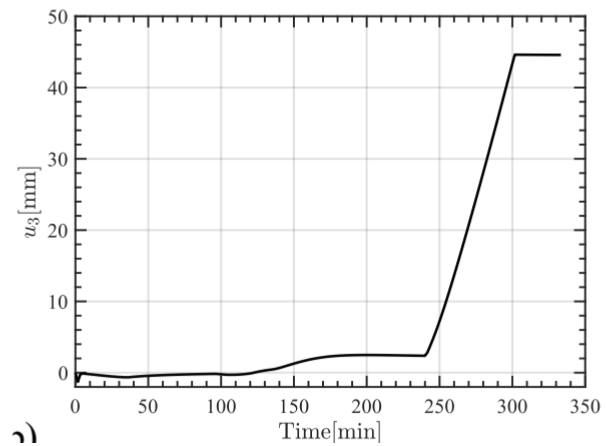




RVE

[45/-45]





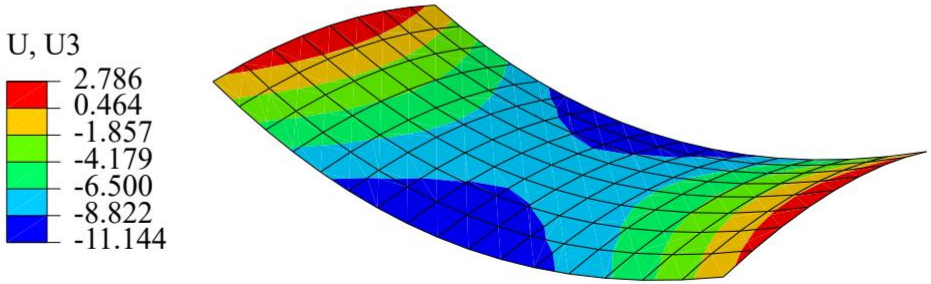
Final deformation (x2)

Deflection of free corner vs time

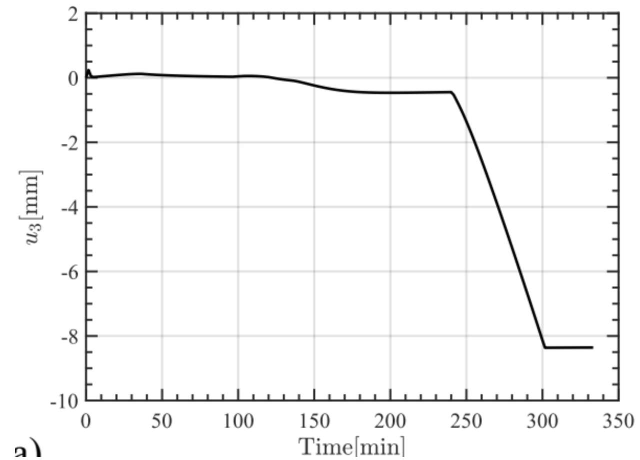
J Zhi, et al., Multiscale modeling of laminated thin-shell structures with Direct FE[2], (2023) CMAME, 407, 115942.

Thermo-mechanical cure-induced deformation

[0/90]

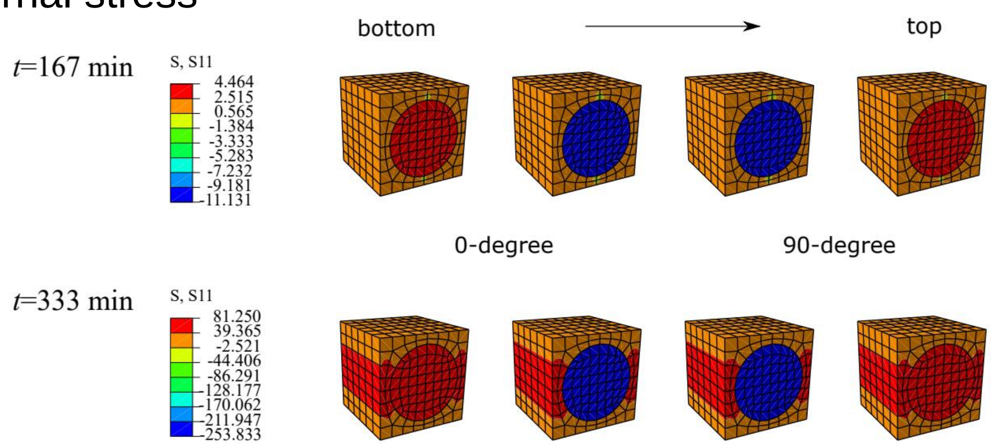


Final deformation (x2)



Deflection of laminate center

Internal stress



Conclusions

- Multiscale simulations can be easily implemented as a single FEA on commercial FE codes with Direct FE^2.
- The implementation is completed at the pre-processing stage. No user intervention is needed thereafter.
- All capabilities of the commercial code, including multiphysics analysis, are available with Direct FE^2.

Thank you!

mpetanbc@nus.edu.sg

DFE2_2to1.py

References

1. Direct FE2 for concurrent multilevel modelling of heterogeneous structures, (2020) CMAME, 360, 112694.
2. A review of the FE2 method for composites, (2021) Multiscale and Multidisciplinary Modeling, Exp and Des, 4 (1).
3. Direct FE2 for simulating strain-rate dependent compressive failure of cylindrical CFRP, (2021) Comp Part C, 5, 100165.
4. Analysis of nonlinear shear and damage behaviour of angle-ply laminates with Direct FE2, (2021) Comp Sci Tech, 216, 109050.
5. Transient multi-scale analysis with micro-inertia effects using Direct FE 2 method, (2021) Comp Mech, 67 (6).
6. Multiscale analysis of thermal problems in heterogeneous materials with Direct FE2 method, (2021) IJNME, 122 (24).
7. Direct FE2 for concurrent multilevel modelling modeling of heterogeneous thin plate structures, (2022) CMAME, 392, 114658.
8. Multiscale computational homogenisation of shear-flexible beam elements: a Direct FE2 approach, (2022) Comp Mech, 70 (5).
9. Direct FE2 modeling of heterogeneous materials with a micromorphic computational homogenization framework, (2022) CMAME, 393, 114837.
10. Multiscale computational homogenisation of shear-flexible beam elements: a Direct FE2 approach, (2022) Comp Mech, 70 (5).
11. Multiscale modelling of sandwich structured composites using Direct FE2, (2023), Comp Sci Tech, 239,110066.
12. Multiscale modeling of laminated thin-shell structures with Direct FE2, (2023) CMAME, 407, 115942.