Computer-aided design of structural parts from short fiber reinforced composites

Andrei A. Gusev

Department of Materials, ETH-Zurich, Switzerland

Outlook

- Structural parts from short fiber composites
- Non-uniform effective properties
- Finite element based procedure for predicting effective properties
- Validation
- Two step orientation averaging approach
- Computer-aided design

Collaboration:

- Dr. P.J. Hine, IRC in Polymer Science & Technology, University of Leeds
- H.R. Lusti, Department of Materials, Polymer Chemistry, ETH Zürich

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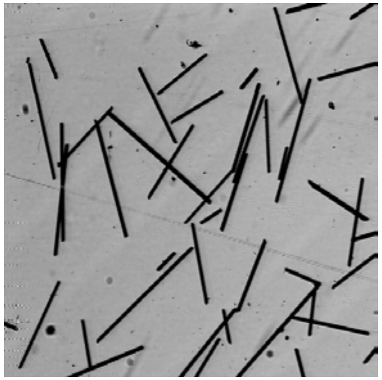
Short fiber composites

- Polymers have a stiffness of 1-3 GPa
  - glass fibers 70 GPa
  - carbon fibers 400 GPa

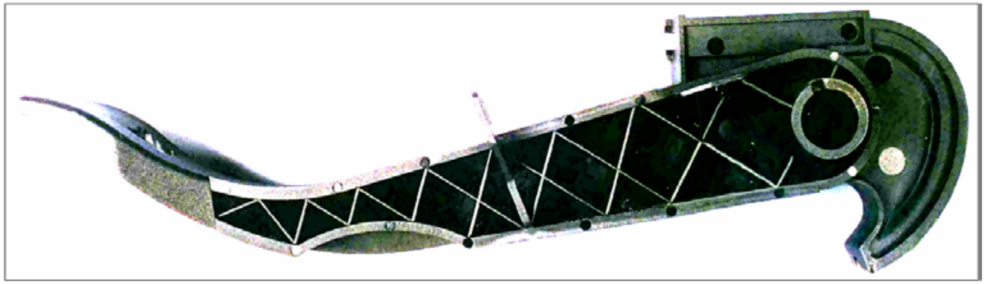
- Short fiber reinforced polymers
  - fiber aspect ratio 10-40
  - volume loading 5-15%



0.5 mm

- Can be processed by injection molding on the same equipment as pure polymers

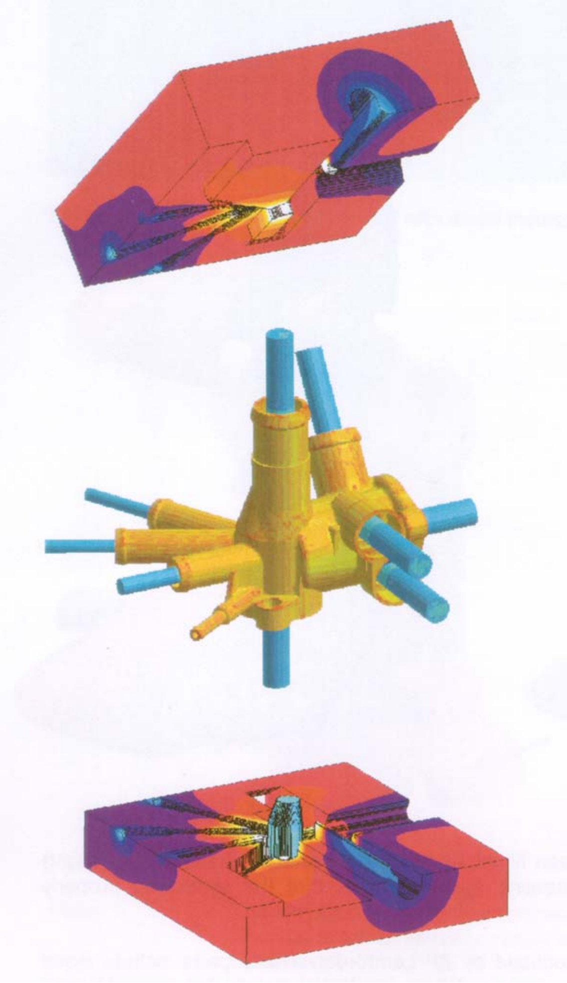
Gear wheel



Acceleration pedal (Ford)

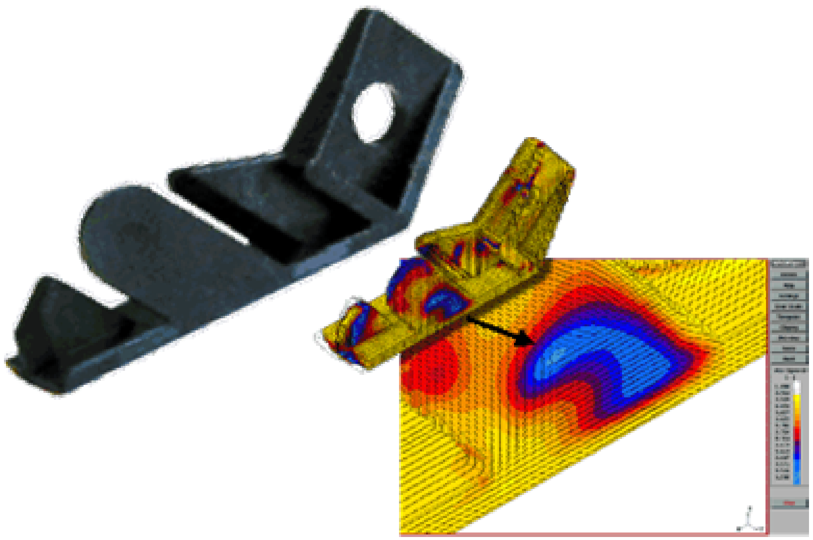
Complex shape parts

- Steel molds (dies) are expensive
  - on the order of $20k and more
- Before any steel mold has been cut
  - mold filling flow simulations
- To optimize mold geometry & processing conditions
  - gate positions
  - flow fronts
  - local curing
  - mold temperatures
  - cycle times
  - etc.
- Software vendors: Moldflow, Sigmasoft, etc.
  - full 3D flow simulations instead of 2½ D
  - 6th order orientation tensor closures



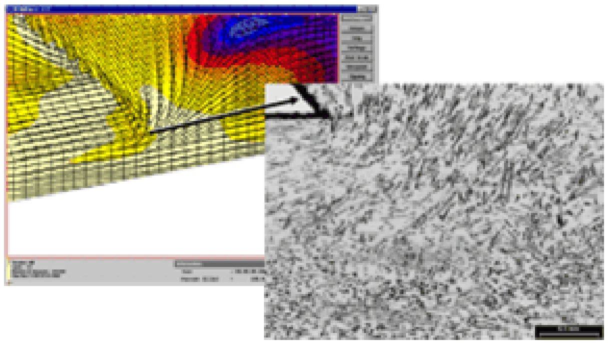
SigmaSoft GmbH, 2001

Local fiber orientation states

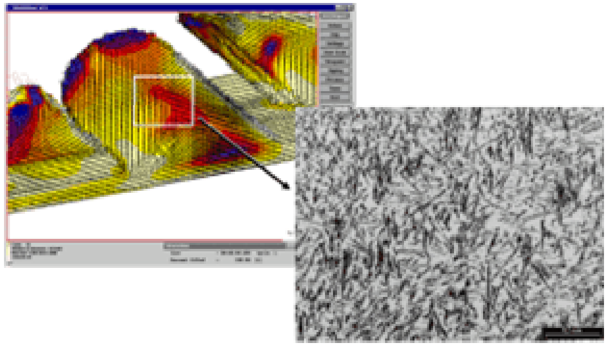


- Non-uniform fiber orientation states
  - ⇒ non-uniform local material properties
    - stiffness
    - thermal expansion
    - heat conductivity, etc.

- Area with a high degree of orientation

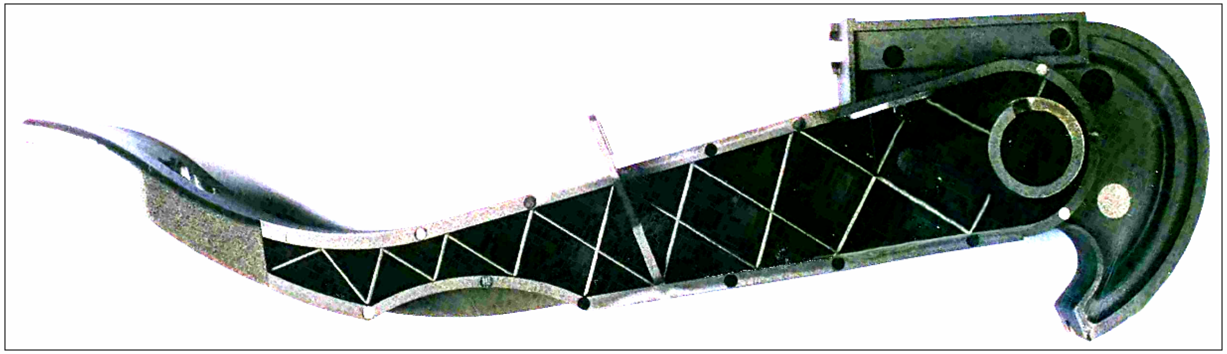


- Area with a low degree of orientation



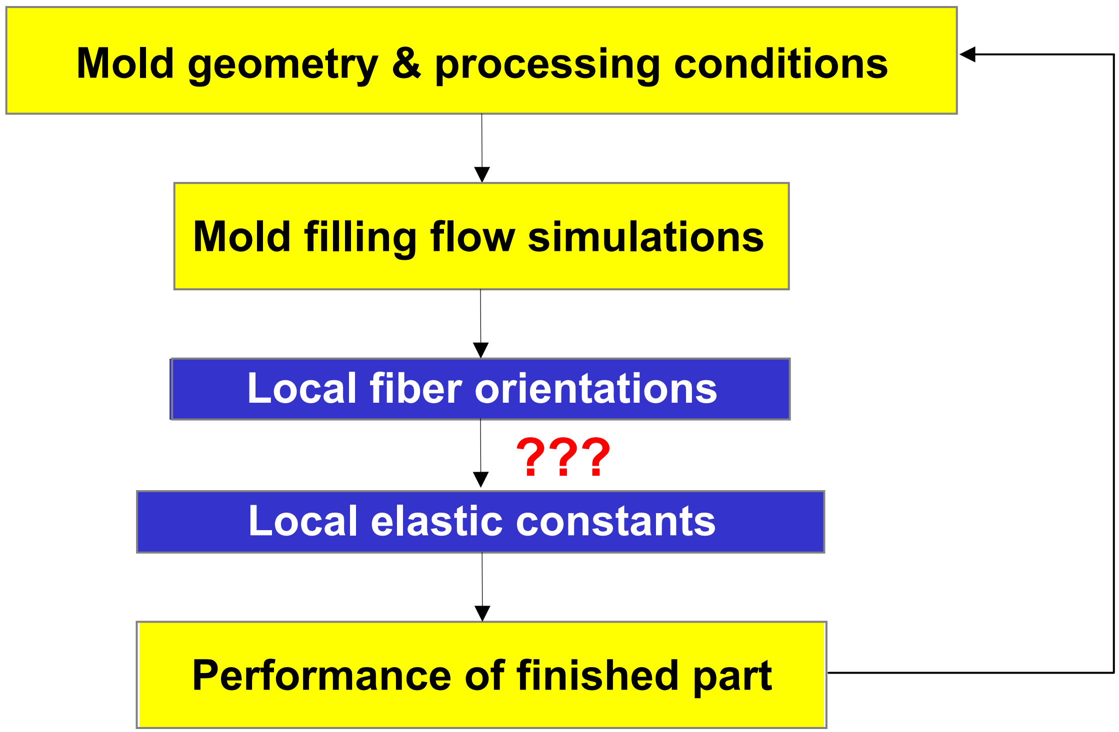
Structural performance

- Finite Element Method
  - software vendors: Abaqus, Ansys, Nastran, etc.
  - only license fees ca. \$1b with a growth rate of 18%



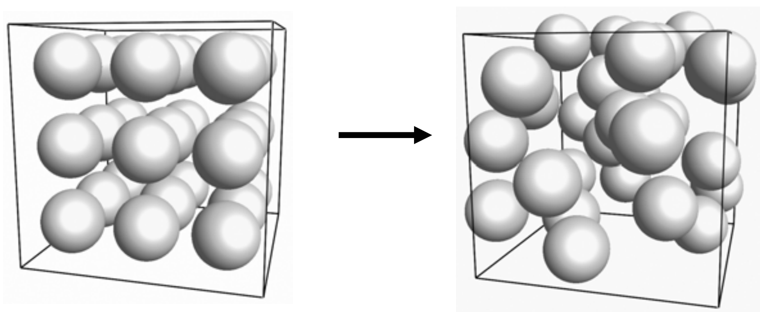
- Short fiber reinforced composite parts
  - mold filling process results in non-uniform fiber orientations
  - and therefore in non-uniform elastic constants
  - in principle, not a problem for FEM
  - provided that the elastic constants across the part are known

Computer-aided design



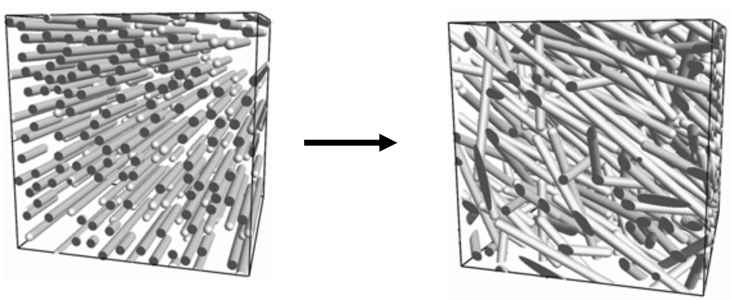
Direct finite element procedure

- Periodic Monte Carlo configurations
  - with non-overlapping spheres



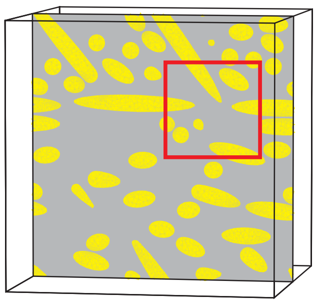
J. Mech. Phys. Solids, **1997**, *45*, 1449

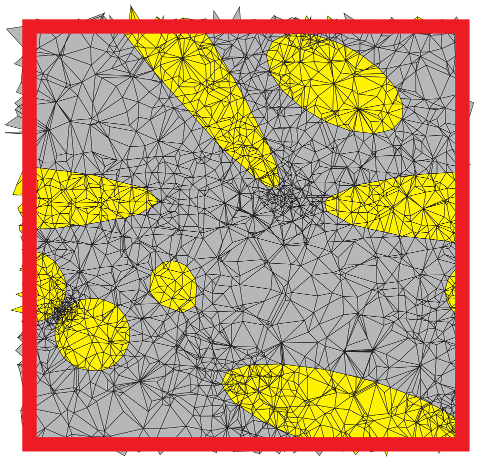
  - with non-overlapping fibers



Adv. Eng. Mater, **2002**, *4*, 933

- Unstructured meshes
  - periodic morphology adaptive





  - 10^7 tetrahedral elements

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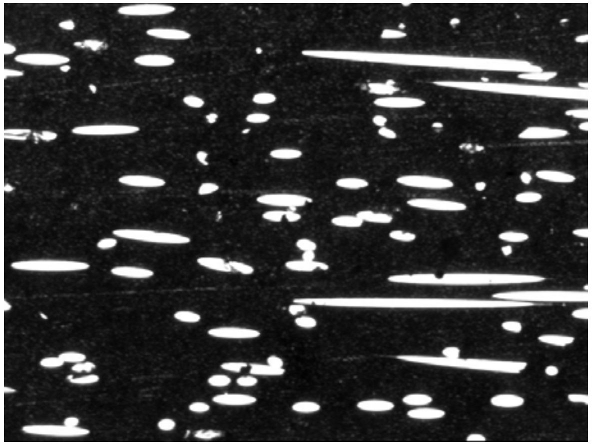
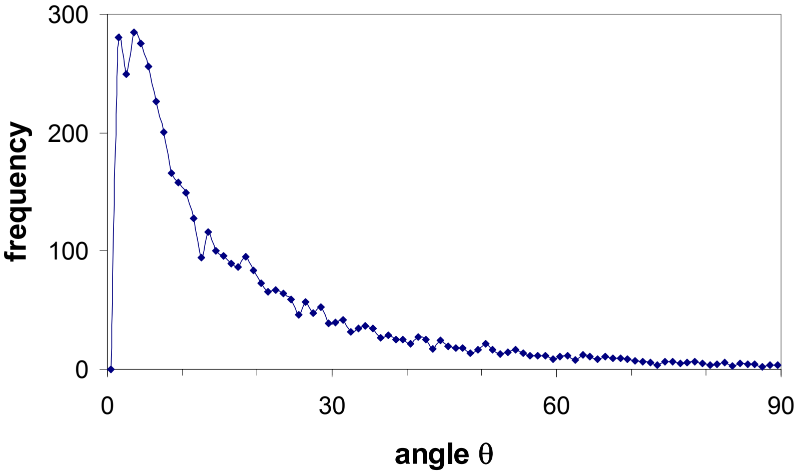
Validation

- Short glass-fiber-polypropylene granulate
  - Hoechst, Grade 2U02 (8 vol. % fibers)
  - injection molded circular dumbbells

- Image analysis
  - typical image frame (700x530 μm)



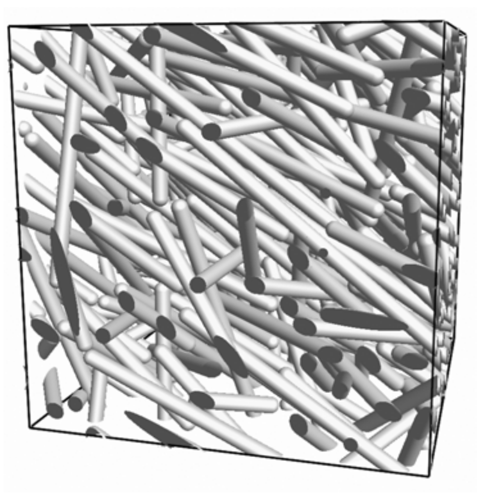
- Measured fiber orientation distribution
  - transversely isotropic
  - statistics of $1.5 \cdot 10^4$ fibers



- Measured phase properties
  - polypropylene matrix
    E = 1.6 GPa, ν = 0.34, $\alpha = 1.1 \cdot 10^{-4}$ K^{-1}
  - glass fibers
    E = 72 GPa, ν = 0.2, $\alpha = 4.9 \cdot 10^{-6}$ K^{-1}
  - average fiber aspect ratio a = 37.3

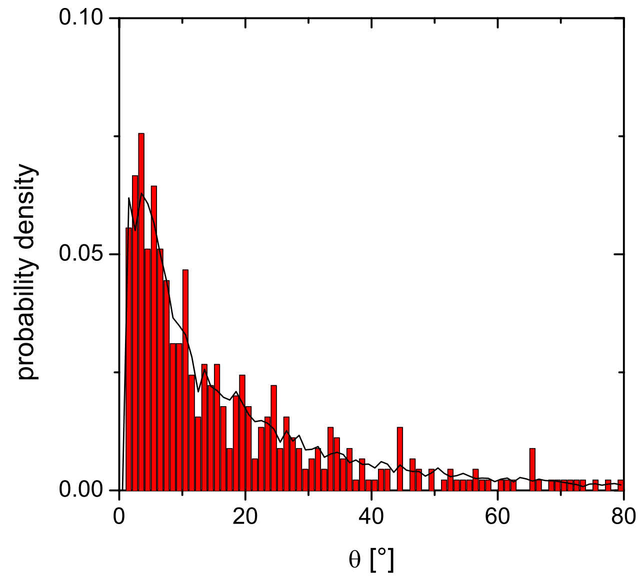
Validation

- Monte Carlo computer models
  - 150 non-overlapping fibers



- AA Gusev, PJ Hine, IM Ward
  Comp. Sci.Tecn. **2000**, *60*, 535
- PJ Hine, HR Lusti, AA Gusev
  Comp. Sci.Tecn. **2002**, *62*, 1927

- Fiber orientation distribution
  - compared to the measured one

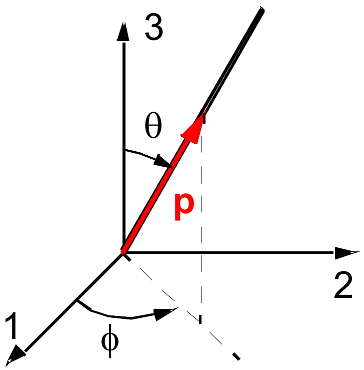


- Effective properties

	numerical	measured
E_{11} [GPa]	5.14 ± 0.1	5.1 ± 0.25
α_{11} $[10^{5}\cdot K^{-1}]$	3.1 ± 0.1	3.3 ± 1.5
α_{33} $[10^{5}\cdot K^{-1}]$	11.7 ± 0.1	12.1 ± 0.2

Two step procedure

- Single fiber
  - unit vector **p** = (p_1, p_2, p_3)

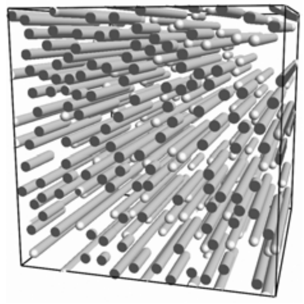


- System with *N* fibers
  - 2nd order orientation tensor

$$a_{ij} = \langle p_i p_j \rangle = \frac{1}{N} \sum_{n=1}^{N} p_i^{(n)} p_j^{(n)}$$

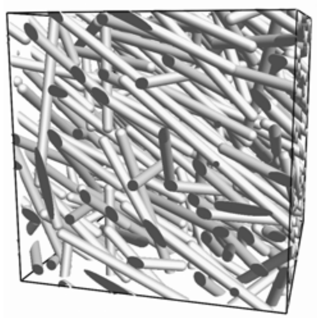
  - 4th & 6th order tensors

- **Step 1:** System with fully aligned fibers



  - numerical prediction for C_{ik}, α_{ik}, ε_{ik}, etc.

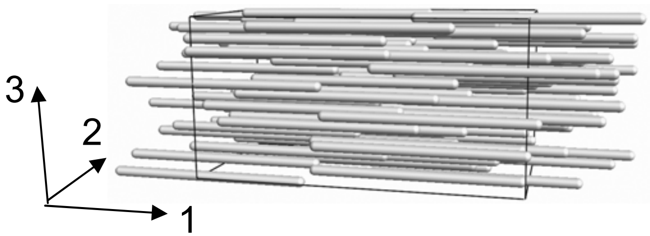
- **Step 2:** System with a given fiber orientation state



  - orientation averaging
  - quick arithmetic calculation

Orientation averaging

- System with fully aligned fibers



  - transversely isotropic
  - effective dielectric constants

$$\begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_2 \end{pmatrix}$$

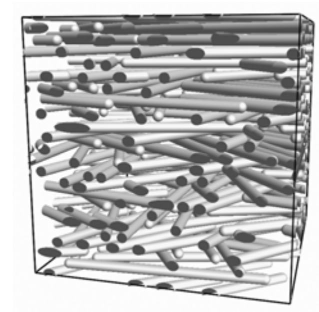
- System with a given orientation state

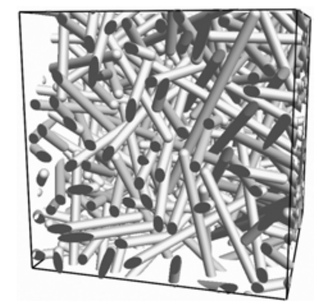
$$\langle \varepsilon_{ij} \rangle_{eff} = (\varepsilon_1 - \varepsilon_2) \cdot a_{ij} + \varepsilon_2 \delta_{ij}$$

  - where δ_{ik} is the unit tensor
  - a_{ik} second order orientation tensor

- Analogous equations for C_{ik}, α_{ik}, etc.
  - with the 4th order orientation tensor

- How accurate are the estimates?





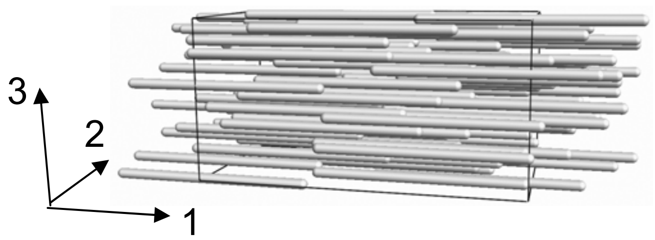
  - about 200 computer models
  - with all possible a_{ik}
  - various fiber loading f and aspect ratio a
  - both glass and carbon fibers

- Remarkably

  direct numerical & orientation averaging agree within 2-3% for both C_{ik}, α_{ik}, and ε_{ik}

Composites with fully aligned fibers

- Empirical Halpin-Tsai equations
  - most widely used in industry
  - initially for long fiber composites
  - then generalized to short fiber ones

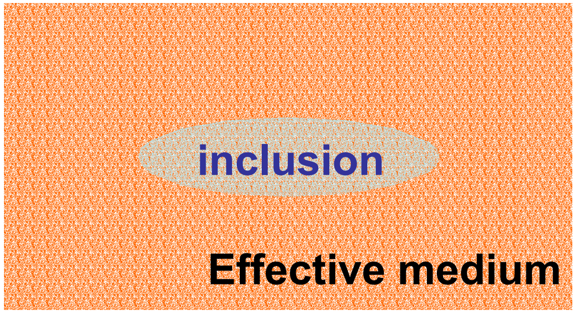


$$\langle E_1 \rangle_{eff} = (1-f)\cdot E_m + f\cdot E_f$$

- Comparison with numerical predictions
  - ca. 100 computer models
  - with different matrices
  - various fiber loading & aspect ratio
  - both glass and carbon fibers

on average ±45%, max.120%

- Rational Tandon-Weng model
  - micromechanics-based
  - single inclusion, self-consistent
  - analytical Eshelby's solution

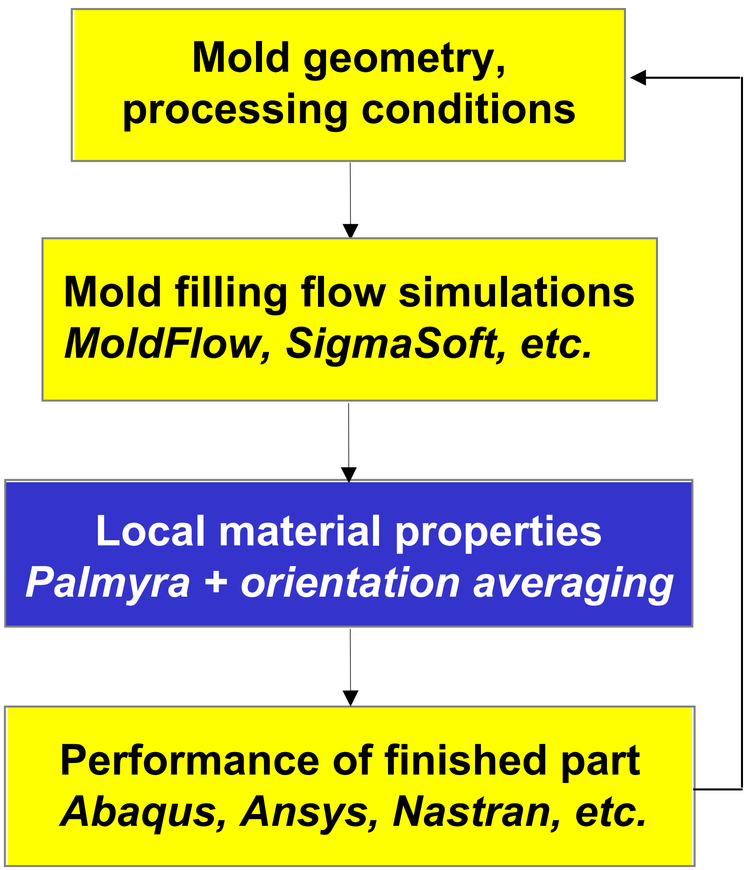


  - closed form solutions for glass fibers
  - Qui-Weng extension to carbon fibers

- Comparison with numerical predictions
  - the same computer models
  - as for the Halpin-Tsai equations

on average ±20%, max. 60%

Computer-aided design of short fiber reinforced composite parts



- Department of Materials
  - Polymer Chemistry
    - Gusev, Hine, Ward, *Comp. Sci.Tecn.* **2000**, *60*, 535
    - Hine, Lusti, Gusev, *Comp. Sci.Tecn.* **2002**, *62*, 1445
    - Lusti, Hine, Gusev, *Comp. Sci.Tecn.* **2002**, *62*, 1927
    - Gusev, Lusti, Hine, *Adv. Eng. Mater.* **2002**, *4*, 927
    - Gusev, Heggli, Lusti, Hine, *Adv. Eng. Mater.* **2002**, *4*, 931
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  - Palmyra by MatSim, www.matsim.ch

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