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BACKGROUND THEORY AND MULTIPOLE EXPANSION TECHNIQUE BASED CODE

AUTHOR:	Dr Volodymyr Kushch
AFFILIATION:	Institute for Superhard Materials NAS of Ukraine
ADDRESS:	2 Avtozavodskaya Str., 04074 Kyiv Ukraine
TEL.:	+38 044 432 9544
EMAIL:	vkushch@bigmir.net
FURTHER AUTHORS:	Sergiy V. Shmegera, Dr Leon Mishnaevsky Jr
REVIEWER:	Project members
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Abstract: The aim of this work is to develop and efficient tool for the computer simulation of progressive damage in the fiber reinforced composite (FRC) materials and thus to provide the micromechanics-based theoretical framework for a deeper insight into fatigue phenomena in them. The unified semi-analytical approach has been developed able to simulate the local stress fields and predict the probable fatigue damage development scenarios at the micro and meso structure scales. The theoretical basis is the Multipole Expansion Method (MEM) proven to be highly efficient way of studying the behavior of large-sized models of composite and suspension mechanics. In this work, it is coupled with the representative unit cell (RUC) model of FRC providing a proper account for the micro structure statistics. A combination of the realistic structure model with the accurate and numerically efficient method of analysis provides probably the most reliable prediction of the composite's behavior.

The developed solving technique combines the superposition principle, the theory of complex potentials, Fourier series expansion and certain new results of the theory of special functions. By using the properly chosen potentials and newly derived re-expansion formulas for them, the model boundary-value problem stated on the multiple-connected domain has been reduced to an ordinary, well-posed set of linear algebraic equations which provides high numerical efficiency of the method. By analytical averaging the strain and stress fields the exact formulae for the effective stiffness tensor have been derived. An accurate solution has been obtained for the micro stress field in a meso cell model of fibrous composite. The model includes several hundred inclusions sufficient to account for the micro structure statistics of composite. The presented numerical examples demonstrate an accuracy and high numerical efficiency of the method which makes it to be a promising tool for studying progressive damage in FRCs. A brief information is provided on the developed Multipole Expansion Method based applied software.

Contents

STATUS, CONFIDENTIALITY AND ACCESSIBILITY										
Status				**Confidentiality**				**Accessibility**	
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PL: *Project leader* **WPL:** *Work package leader* **TL:** *Task leader*

1. The meso cell model of fiber reinforced composite (FRC)

1.1. *Model geometry*

The meso cell model of the FRC bulk, shown in Fig.1.1, represents the next step in development of the "finite array of inclusions" model studied by Kushch et al. (2005) and Buryachenko and Kushch (2006). Namely, we consider a quasi-random model structure, respectively, a unit cell of which contains a certain number of aligned and circular in cross-section fibers. Within a cell, the fibers are placed arbitrarily but without overlapping. The fibers with edges shown in Fig. 1.1 by dashed line do not belong to the cell while occupying a certain area within it. Geometry of the cell is given by its length and height, the coordinates of the centers of fibers and their radii. The composite bulk is obtained by translating the cell in two orthogonal directions. Number of the fibers with centers inside the cell is taken large sufficiently to approach micro geometry of an actual disordered composite. Diameter and the elastic moduli are defined individually for each separate fiber. It provides applicability of this model for studying the multi-component systems and the effect of fiber diameter scattering, which are quite considerable in the commercial FRCs (Babuška et al., 1999).

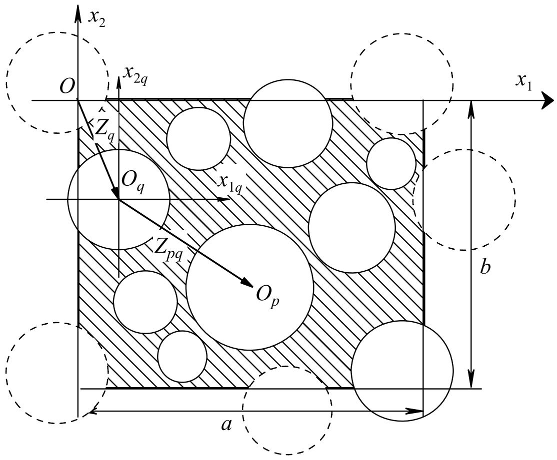

Fig. 1.1. Geometry model of the composite bulk

The structure model (Fig. 1.1) of statistically homogeneous quasi-random composite is generated by the molecular dynamics algorithm of growing particles (Sangani and Yao, 1988) with subsequent equilibrization to guarantee reproducible thermodynamic properties of the model (Torquato, 2002). In Fig. 1.2, the empirical radial distribution function for the model FRC with N=100 and volume content of fibers c=0.65 is shown. The open circles represent data for a single structure realization, solid circles are obtained by averaging over 10 runs. The solid and dash-dotted lines show the analogous data obtained by Truskett et al. (1998) and Buryachenko et al. (2003), respectively. As seen from the plot, our data practically coincide with the results by Truskett et al. (1998) which validates the developed by us algorithms and software.

The following modification of the above model is also of practical interest. In Fig. 1.3a, a typical structure of cross-ply FRC laminate is shown. Babuška et al. (1999) have reported considerable local decrease of the fiber volume content and stress re-distribution in a vicinity of the inter-ply boundary. The adequate model of composite ply is shown in Fig. 1.4: it differs from the "bulk model" in that no fiber intersections with the flat edges of the ply are allowed. This model makes possible studying the edge effects caused by the low fiber volume content nearby the ply boundary and by interacting with the neighboring plies provided the boundary conditions at the flat edges were properly stated. The developed method is applied equally to both these models. Noteworthy, the model we consider involves the additional structure parameter, namely ply thickness, so it can be thought as a meso level model. Also, it seems reasonable to regard the typical damage observed in Fig. 1.3b as the meso level event rather than micro- or macroscopic ones associated with a single fiber and entire composite part, respectively. Due to these reasons, we will call our model as a "meso cell"; for more discussion on the subject, see Mishnaevsky (2007).

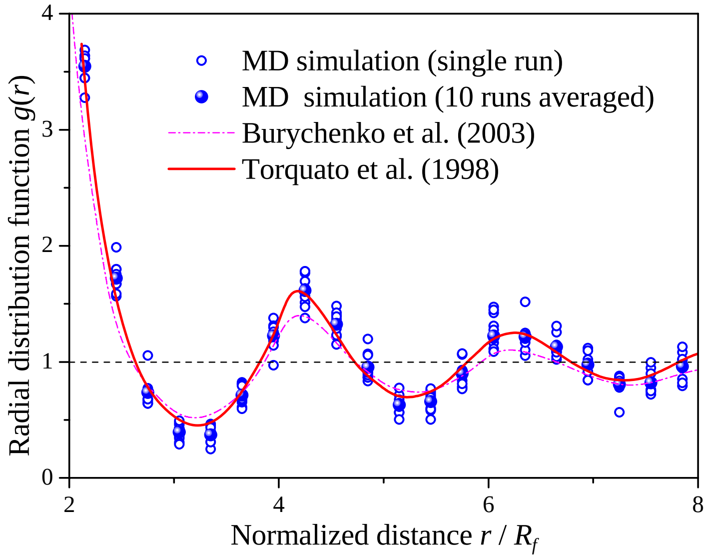

Fig. 1.2. Radial distribution function of the quasi-random composite cell model: 100 fibers per cell, solid line is obtained by averaging over 10 realizations

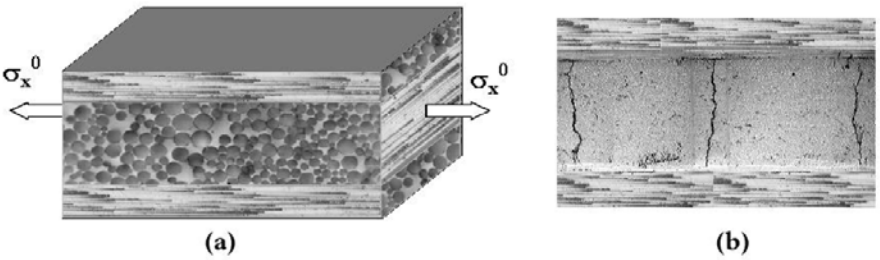

Fig. 1.3. Cross-ply laminate (a) subjected to uniaxial loading and (b) resulting damage (Joffe, 1099).

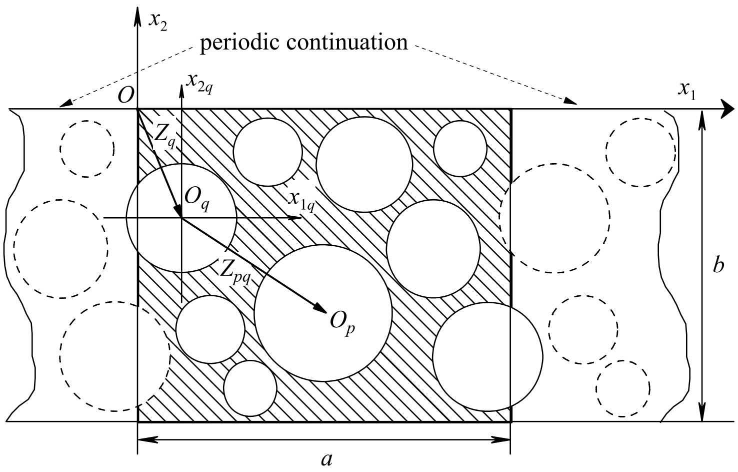

Fig. 1.4. Structure model of the composite ply

1.2. *Model boundary value problem (BVP)*

Within the 2D framework, the (a) plane strain, (b) plane stress and (c) anti-plane shear problems for FRC model are studied. Both the matrix and fiber materials are isotropic and linearly elastic. At the matrix-fiber interfaces, the perfect bonding conditions (continuity of displacements and normal tractions) are prescribed:

$$\left(u_m - u_i^{(q)}\right)\Big|_{r_q = R_q} = 0; \qquad \left[\tau_n(u_m) - \tau_n(u_i^{(q)})\right]\Big|_{r_q = R_q} = 0;$$
$$q = 1,\ 2,\ \ldots,\ N;$$

The stress field in the composite bulk is assumed to be macroscopically homogeneous, which means constancy of the volume-averaged, or macroscopic, strain $\varepsilon^*{}_{ij} = \langle \varepsilon_{ij} \rangle$ and stress $\sigma^*{}_{ij} = \langle \sigma_{ij} \rangle$ tensors, which are considered in a given context as the governing parameters. The far field load defined by the macroscopic strain tensor is typical in the homogenization problem where the macroscopic, or effective, moduli are to be determined. On the contrary, using the macroscopic stress tensor as the load governing parameter is preferable in the local stress concentration study. Under macroscopic stress homogeneity condition periodicity of structure results in periodicity of relevant physical fields. The stress periodicity

$$\sigma_{ij}(z+a) = \sigma_{ij}(z+\mathrm{i}b) = \sigma_{ij}(z)$$

can be alternatively regarded as the cell boundary condition providing continuity of the displacement and stress fields between the adjacent cells. The relevant decomposition of displacement field involves the linear part being the far field and the periodic fluctuation caused by the inhomogeneities..

1.3. *Analytical method*

An accurate analytical method has been developed to solve for stress in the meso cell comprising

- the Muskhelishvili's (1953) complex variables technique;
- the superposition principle;
- the Golovchan et al. (1993) singular periodic potentials;
- the Fourier and Laurent series and
- the newly derived re-expansion formulae.

The solution of the model BVP is built in a computationally cost-efficient way, in the class of periodic functions rather than doubly-periodic ones in conventional multipole expansion method (e.g., Movchan et al, 1997). By complete fulfilling all the boundary conditions, the model BVP is reduced to the well-posed infinite set of linear algebraic equations with the matrix coefficients given by rational expressions and involving (unlike FEM or BEM) no integration. It provides high numerical efficiency of the method. It is of primary importance in the progressive damage we aim to study because, in order to simulate the complete path of successive damage, one must solve the model BVP repeatedly several tens or even hundreds times. The developed method is sufficiently flexible to consider the both "composite bulk" and "composite ply" models with an adequate account for the edge effects. The stress field obtained from the above solution is integrated analytically to get the closed form exact expressions of the effective, stiffness tensor.

The analytical formulas of the method are rather involved and too lengthy to be reproduced here. For the details of derivation in the isotropic case, see the papers by Kushch et al. (2008a) and Sevostianov and Kushch (2009). Generalization of the method on the case of fibrous composite with anisotropic constituents is given by Kushch et al. (2008b). A detailed full account of the method is given in the *UpWind ISM Annual Report-2007*.

2. Numerical testing

2.1. Numerical realization and efficiency

The derived series solution is asymptotically exact. Its numerical algorithm involves the truncation procedure (retaining a finite number N_{eqn} of equations and unknowns) and provides any desirable accuracy of solution by the appropriate choice of N_{eqn}. High efficiency of numerical scheme stems from the fact that the method deals with simple rational expressions and ordinary rapidly convergent sums only and - unlike FEM or BEM - involves no integration. The most computational time is spent by the linear solver: the generalized minimum residuals (GMRES) algorithm by Saad and Schultz (1986) has been chosen as the best compatible with the multipole expansion technique. Convergence rate (and hence numerical efficiency) of GMRES depends on the rational choice of preconditioner matrix and initial guess. Following Fu et al. (1998), the block-Jacobi preconditioner is chosen which has a clear physical meaning for the many-inclusion problem (i.e., solution for non-interacting fibers).

Table 2.1. Linear Solver Elapsed Time, s

N_{eqn}	DLAX	DLSARG	GMRES
1600	9.5	3.0	0.43
2400	31.9	8.6	0.94
3600	79.1	40.5	1.8
4800	lost accuracy	100.1	4.2

The open source Fortran code of GMRES routine by Fraysse et al. (1998), with minor modifications, is utilized. Its performance is seen from Table 2.1, where the run time vs number of equations N_{eqn} is given for three double precision linear solvers. They are: DLAX, standard direct solver (SSL2 library, Lahey Fortran 5.7); DLSARG, standard direct solver (IMSL library, Compaq Visual Fortran 6.5) and GMRES, the problem-adjusted iterative solver. All the subsequent numerical data have been obtained using the Pentium IV 2.4 GHz single processor PC. It is seen from the Table that using the standard direct solvers have no perspective. Yet another argument in favor of iterative solver for the progressive damage simulation consists in that the solution obtained on the previous step is an initial guess for the next step: doing so results in the rapid convergence of iterations. The further improvement of numerical efficiency can be achieved by taking more elaborated preconditioner and by allowing the algorithm to automatically adjust the number of terms in Fourier series in order to reach the desirable level of accuracy.

2.2. Convergence

Three main parameters governing convergence and accuracy of results in the statistical analysis are

- number N_{harm} of harmonics retained in the series expansions;
- number N_{fib} of fibers with the centers lying inside the unit cell;
- number N_{conf} of random structure realizations taken for averaging.

All these numbers should be taken sufficiently large to provide the reliable numerical results. On the other hand, computational effort of our study scales as $(N_{eqn})^2\ N_{conf}$, where number of equations $N_{eqn} = 4\ N_{fib}\ N_{harm}$ and, to avoid exceedingly large total computational time, the reasonable values of N_{harm}, N_{fib} and N_{conf} are to be taken. Their motivated choice is based on the solution convergence rate study.

First, we evaluate number of harmonics N_{harm} we need to keep in the numerical solution in order to get the convergent solution. The convergence rate is seen from Tables 2.2 and 2.3, where the peak interface stress $\sigma_{r\,max} = \max \sigma_r$ is given as a function of δ_{min} and N_{harm}.

Table 2.2. $\sigma_{r\,max}$ at interface: two inclusions along the loading direction

N_{harm}	δ_{min}			
1	0.5	0.2	0.05	0 .02
10	2.00	2.75	4.32	26.3
20	2.00	2.76	4.25	5.55
30	2.00	2.76	4.25	5.19
40	2.00	2.76	4.25	5.18

Table 2.3. $\sigma_{r\,max}$ at interface: a square array of inclusions

	δ_{min}			
N_{harm}	0.5 (c = 0.349)	0.2 (c = 0.545)	0.05 (c = 0.712)	0.02 (c = 0.755)
10	1.53	1.74	2.88	2.26
20	1.53	1.72	2.29	2.66
30	1.53	1.72	2.28	2.69
40	1.53	1.72	2.28	2.70

The data shown in Table 2.4 were obtained for the random structure realization (30 inclusions per cell) with δ_{min} = 0.02; the fiber volume content c is taken the same as in Table 2.3.

Table 2.4 $\sigma_{r\,max}$ at interface of the arbitrarily chosen fiber: quasi-random array of inclusions

N_{harm}	c = 0.349	c = 0.545	c = 0.712	c = 0.755
10	8.00	5.36	5.38	6.47
20	3.90	3.50	2.59	2.73
30	3.88	3.50	2.57	2.72
40	3.88	3.50	2.57	2.72

Here, no smooth $\sigma_{r\ max}$(c) dependence is expected because, for each c, only one random structure realization was taken. However, the max stress decreasing tendency is quite clear: the higher is the fiber volume content, the less room left for isolated clusters of a few fibers where the highest interface stress concentration is most probable.

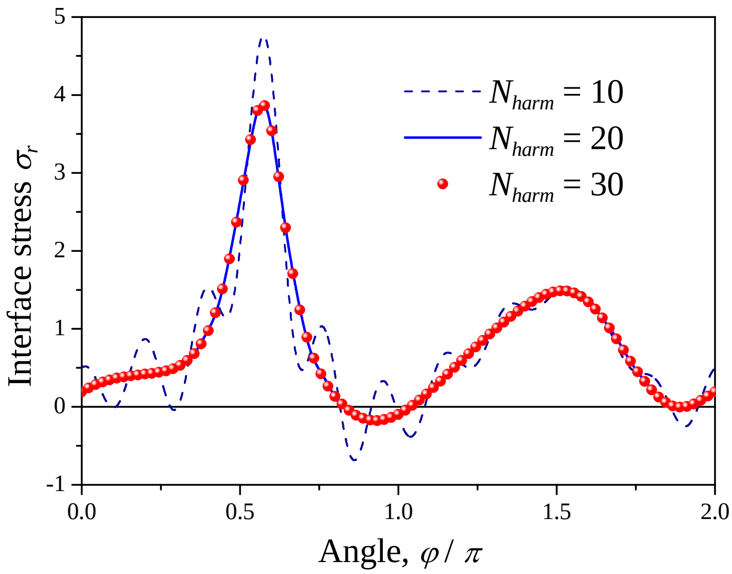

Fig. 2.5. Interface stress convergence with N_{harm} increased

In Fig. 2.5, the σ_r stress variation along the interface of the arbitrarily chosen fiber in the model with 30 fibers per cell, c = 0.349 and δ_{min} = 0.02. The stress convergence is uniform and already N_{harm} = 20 gives the practically convergent solution with a relative error in stress below 1%. The smaller δ_{min} is, the stiffer the model BVP is and the higher local stress concentration is expected. By taking a fixed allowable distance δ_{min}, we pre-determine the maximum allowable stress and hence this parameter should be taken as small as possible. An idea of how $\sigma_{r\,max}$ is affected by δ_{min} can be drawn from the stress asymptotics for nearly touching fibers.

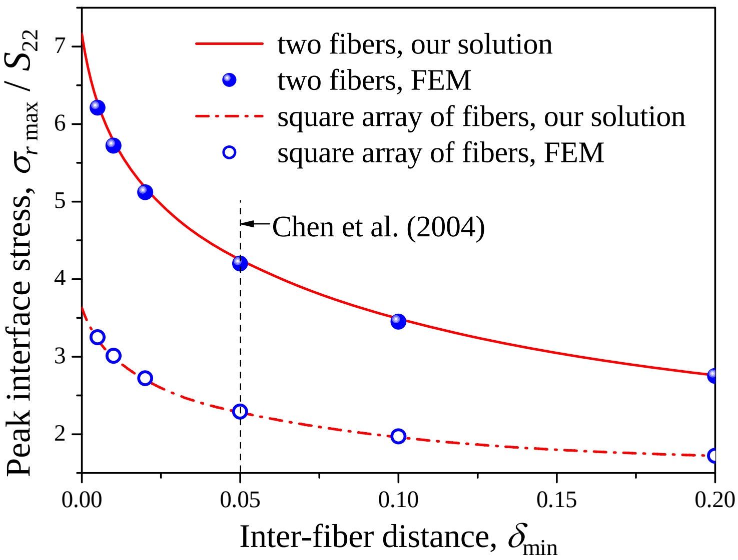

Fig. 2.6. Peak interface stress $\sigma_{r\,max}$ as a function of normalized inter-fiber distance

The developed analytical method is also advantageous in that it, BEM and FEM unlike, handles equally well the problems with separated and touching inclusions. It is seen from Fig 2.6 that the interface stress remains finite when the fibers are drawn together ($\delta_{min} \to 0$): the stress singularity is expected only in the case of rigid (non-deformable) inclusions. The lines represent our solution, the analogous data obtained by FEM are shown in the plot by the solid circles for two fibers and by the open circles for a square array of fibers. The compared data practically coincide which validates both the developed theory and numerical code. For δ_{min} = 0.05 adopted by Chen and Papathanasiou (2004) the probable $\sigma_{r\,max}$ underestimation is almost two times. The value δ_{min} = 0.01 seems to be a reasonable compromise between the accuracy and computational effort.

The next issue is a number of fibers N_{fiber} inside the unit cell. The data in Table 2.5 are the mean stress inside the cell, averaged over 50 configurations. Taking account of that loading is the uniaxial macroscopic strain E_{kl} = 1, these numbers are also the effective elastic moduli of a fibrous composite C^*_{ijkl} .

Table 2.5. Effective stiffness of a fibrous composite: convergence and isotropy checking

	σ_{11}/C_{1111}	σ_{22}/C_{2222}	σ_{12}/C_{1212}
N=20, E_{11}=1	2.685 ± 0.016	2.242 ± 0.012	0.009 ± 0.012
N =20, E_{22}=1	2.242 ± 0.011	2.659 ± 0.016	0.009 ± 0.012
N =50, E_{11}=1	2.683 ± 0.011	2.270 ± 0.008	-0.006 ± 0.008
N =50, E_{22}=1	2.271 ± 0.008	2.671 ± 0.010	-0.005 ± 0.009

It is seen from the Table that the values obtained for N_{fib} = 20 and N_{fib} = 50 are rather close which clearly indicates convergence of solution with respect to N_{fib}. These data are also useful in verifying isotropy of the random structure model. Ideally, one must get for macroscopically isotropic composite material. As calculations show, already for N_{fib} = 20 an anisotropy degree is below 1% and shows a tendency to decrease with the N_{fib} growing up.

Fig. 2.7 shows how much a number of realizations N_{conf} affects the results of statistical averaging. Here, the normalized effective Young modulus E_{eff}/E_0 averaged over a number of random structure realizations is shown. The open circles correspond to N_{fib} = 20 whereas the solid circles correspond to N_{fib} = 50. Based on these observations, the conclusion can be drawn that N_{conf} = 50 provides practically convergent solution.

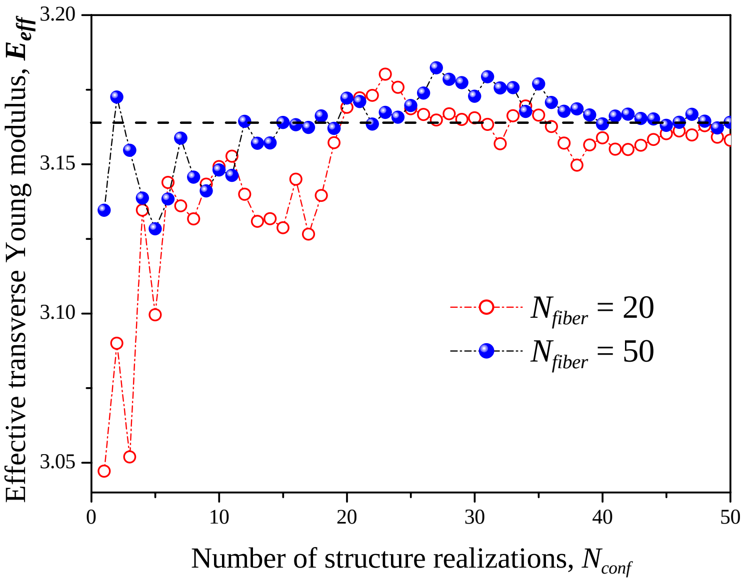

Fig. 2.7. Convergence of effective transverse Young modulus of FRC with a number of realizations N_{conf} increased

Noteworthy, these data must be considered only as the indicative ones as they depend on the volume content of fibers, fiber-to-matrix moduli ratio, microstructure type, etc. In each specific case, a similar testing must be done and the appropriate numbers ensuring the accurate and statistically meaningful results should be determined.

3. Multipole Expansion Method based software

Based on the above mentioned algorithms, the Windows XP/2000 software product COMPOSITE MESOCELL has been developed. The numerical routines are written in Fortran 95, for visualization of the input and output data, the OpenGL graphical library has been utilized. The total length of source code is about 7000 Fortran lines, or 325 Kbytes. The program is interactive and provides a set of menus and dialogs for the problem specification, input the problem data, monitoring the flow of solution and post-processing the output data. Also, it contains several additional options providing control of the run flow and visualization process. The software provides the extended possibilities of adjusting the existing problem formulation, checking and correcting the structure model, allows to choose between the problems to be solved, to evaluate the empirical RDF of model composite and to perform the detailed study the stress field in the matrix, fibers and at the interfaces.

The problem dialog shown in Fig. 3.1, defines the problem and loading type and the value of far load, the volume content of fibers, the elastic properties of matrix and fiber materials, etc. Also, there shown a typical representative unit cell of composite the model problem is stating for. For generation of the quasi-random model structure, the described above Molecular Dynamics based packing algorithm is utilized. The main computational algorithm of the program implements the developed version of the Multipole Expansion solving technique and involves

(a) evaluation of the lattice sums entering the matrix coefficients of the resolving linear set of equations, (b) its solution using the iterative GMRES linear solver (c) evaluation of the local stress fields and the macroscopic, or effective, elastic moduli of FRC. An opportunity is provided of one-time solution (prefect interface option) or step-by-step progressive damage simulation regime, where the problem is solved iteratively, with the removing on each step of the fibers based on that or another debonding criterion.

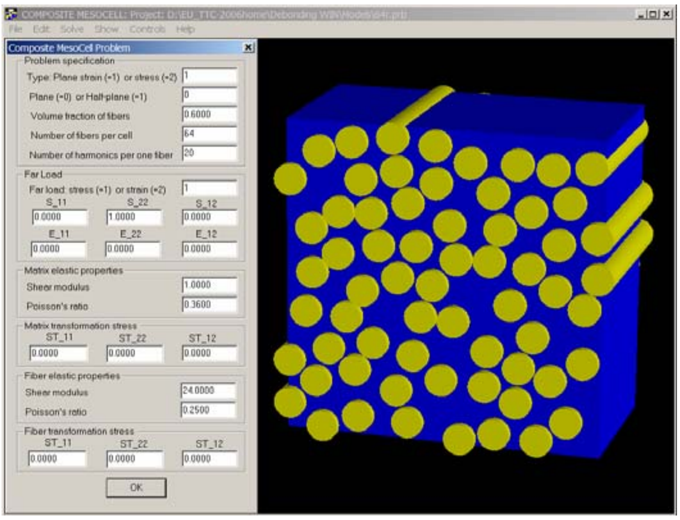

Fig. 3.1. Representative unit cell model and problem dialog

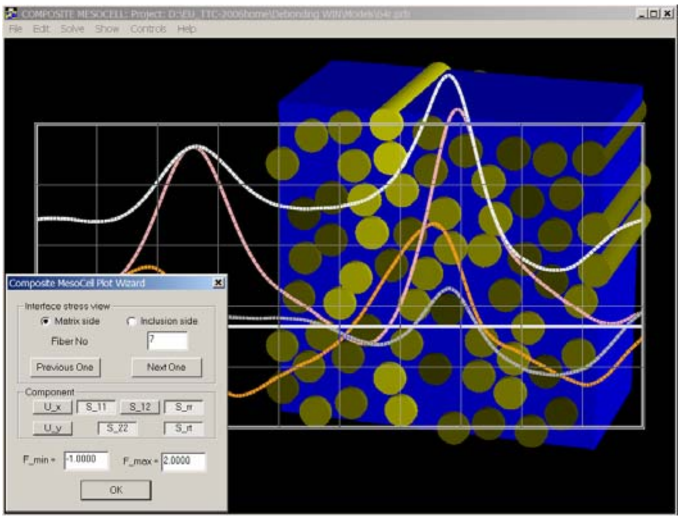

Fig. 3.2. Output DataViewer: interface stress analysis

Visual interactive post-processing is shown in Fig. 3.2, where the Output DataVeiwer is seen as well as the plots of stress variation along the matrix-fiber interface. The colored fibers in the cell model illustrate distribution of the max interface stress: it is easily seen that the heavily loaded fibers, marked by light yellow color, form the chains. The results of numerical study performed with aid of the COMPOSITE MESOCELL software have been reported by Kushch et al. (2008a) and Kushch et al. (2008b).

4. Conclusions

An accurate analytical method has been developed to solve for stress in an infinite quasi-random array of circular inclusions embedded in the matrix, the last being a "meso cell" model of disordered fibrous composite. Up to several hundred of interacting fibers can be considered in the model which is sufficient to account for the micro structure statistics of a real composite. The method combines technique of periodic complex potentials with the Fourier series expansion and re-expansion formulae and can be thought as a version of the multipole expansion method. The developed theory and algorithms reduce the primary boundary-value problem of the elasticity theory for a multiple-connected domain to an ordinary well-posed set of linear algebraic equations. Together with the properly chosen iterative solver, it provides high numerical efficiency of the method, which makes it potentially efficient tool for studying progressive damage in FRCs.

References:

1. Babuška, I., Andersson, I., Smith, P.J., Levin, K., 1999. Damage analysis of fiber composites Part I: Statistical analysis on fiber scale. Comput. Methods Appl. Mech. Engrg. 172, 27--77.
2. Buryachenko, V.A., Kushch,V.I., 2006. Effective transverse elastic moduli of composites at non-dilute concentration of a random field of aligned fibers. Z. angew. Math. Phys. (ZAMP) 57, 491--505.
3. Buryachenko, V.A., Pagano, N.J., Kim, R.Y., Spowart, J.E., 2003. Quantitative description and numerical simulation of random microstructures of composites and their effective elastic moduli. International Journal of Solids and Structures 40, 47--72.
4. Chen, X., Papathanasiou, T.D., 2004. Interface stress distributions in transversely loaded continuous fiber composites: parallel computation in multi-fiber RVEs using the boundary element method Composites Science and Technology 64, 1101--1114.
5. Fraysse, V., Giraud, L., Gratton S., 1998. A Set of Flexible-GMRES Routines for Real and Complex Arithmetics. CERFACS Technical Report TR/PA/98/20.
6. Fu, Y., Klimowski, K.J., Rodin, G.J. et al., 1998. A fast solution method for three-dimensional many-particle problems of linear elasticity. Int. J. Numer. Meth. Engng. 42, 1215--1229.
7. Golovchan ,V.T., Guz, A.N., Kohanenko, Yu., Kushch, V.I., 1993. Mechanics of composites (in 12 volumes). Vol.1. Statics of materials. Naukova dumka, Kiev.
8. Joffe, R., 1999. Damage accumulation and stiffness degradation in composite laminates. PhD thesis, Lulea University of Technology, Lulea, Sweden.
9. Kushch, V.I., Shmegera, S.V., Buryachenko, V.A., 2005. Interacting elliptic inclusions by the method of complex potentials. International Journal of Solids and Structures 42, 5491--5512.
10. Kushch V.I., Shmegera S.V., Mishnaevsky L. Jr, 2008a. Meso cell model of fiber reinforced composite: Interface stress statistics and debonding paths. International Journal of Solids and Structures 45, 2758—2784.
11. Kushch, V.I., Shmegera S.V., Mishnaevsky L. Jr, 2008b. Stress concentration and effective stiffness of aligned fiber reinforced composite with anisotropic constituents. International Journal of Solids and Structures 45, 5103--5117.
12. Movchan, A.B., Nicorovici, N.A., and McPhedran, R.C., 1997. Green's Tensors and Lattice Sums for Elastostatics and Elastodynamics. Proceedings of the Royal Society, A 453, 643-662.
13. Muskhelishvili, N.I., 1953. Some basic problems of the mathematical theory of elasticity. Groningen, P. Noordhoff.
14. Saad, Y., Schultz, M.H., 1986. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. SIAM J. Sci. Stat. Comput. 7, 856--869.
15. Sangani, A.S., Yao, 1988. Bulk thermal conductivity of composites with spherical inclusions. Journal of Applied Physics 63, 1334-1341.
16. Sevostianov, I., Kushch, V.I. Effect of pore clusters on the statistics of peak stress and overall properties of porous material. *International Journal of Solids and Structures* 46 (2009) 4419–4429
17. Torquato, S., 2002. Random Heterogeneous Materials: Microstructure and Macroscopic Properties, Springer-Verlag, New York.
18. Truskett, T.M., Torquato, S., Sastry, S., Debenedetti, P.G., Stillinger, F.H., 1998. Structural precursor to freezing in the hard-disk and hard-sphere systems. Physical Review E 58, #3 3083-3088.