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Trefftz radial basis functions (TRBF)

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The TRBF's are radial functions satisfying governing equation in the domain. They can be used as interpolation functions of the field variables especially in boundary methods. In present paper discrete dipoles are used to simulate composite material reinforced by stiff particles using with boundary point collocation method which does not require any meshing and any integration. The better the interpolation function satisfies also the boundary conditions, the more efficient it is. In examples it is shown that a triple dipole (which is a TRBF) located into the center of the particle can approximate the inter-domain boundary conditions very good, if the particles are not very close to each other and their size is not very different. In general problem the model can be used as very good start point for international improvements in refined model. Composite reinforced by short fibres with very large aspect ratio continuous TRBF were developed. They enable to reduce problem considerably and to simulate complicated interactions for investigation such composites.

Keywords: fibre reinforced composites, meshless method, Trefftz Radial Basis Functions, continuous source functions

1. Introduction

In computational simulations, boundary-type solution methodologies are now well established as alternatives to prevailing domain-type methods such as FEM, because of the computational advantages they offer by way of reduction of dimensionality, good accuracy for the whole domain, and simplicity of data preparation for the model. Using the virtual boundary method and radial basis functions (RBF), the boundary point collocation method has been proposed to construct a boundary meshless formulation [27, 28], in which the boundary conditions and body forces are enforced and coupled with the analogue equation method to construct a boundary-type meshless method for analyzing nonlinear problems [29].

The method of fundamental solutions [5, 11] (MFS) is a boundary meshless method which does not need any mesh. In linear problems, only nodes (collocation points) on the domain boundaries and a set of source functions (fundamental solutions) in points outside the domain are necessary to satisfy the boundary conditions. MFS has certain advantages over the BEM, as it completely avoids the need for any integral evaluation and it leads to very simple formulations in some problems. However, large numbers of both collocation points and source functions are necessary if the shape of the domain is complex and moreover, the resulting system of equations is bad conditioned in some problems. The source functions serve as the trial functions and must be placed outside the domain. The location of the source functions is vital to both the accuracy and the numerical stability of the solution. The MFS can be also included among Trefftz-type (T-) methods [9, 26].

The fast multi-pole method [4, 6, 7, 16, 18, 20, 21, 23] (FMM) was developed to increase the efficiency of the boundary type numerical models by reducing computations for the interaction of far fields. However, near field integrals still have to be solved by classical BEM and the boundaries are also discretized by elements. The FMM improves considerably numerical models based on the BEM especially for far field interaction. However, the near field interaction is solved by classical procedure and the models for composites reinforced by many interacting fibres and particles require still very efficient computers.

In our presentation we will show how the Trefftz Radial Basis Functions (TRBF), i.e. RBF satisfying the governing equations (which can be the fundamental solutions, or more general functions, dipoles, dislocations, etc.) can be used to increase the efficiency of simulations. The most efficient methods will be those which will best approximate both domain variables and boundary conditions. The TRBF are source functions having their source points outside the domain. Special attention will be given to application of the TRBF in the form of dipoles to the simulation of composites reinforced by particles and/or short fibres. We don't understand the TRBF to be a method of solution, but it is a tool of approximation of field variables and they can be used in different forms for solution of problems. Discrete and 1D continuous distribution TRBF are shown in application to the simulation of the interaction of the particles/fibres with matrix. In this way a variation of interpolation functions can be obtained in order to satisfy the inter-domain boundary conditions.

Not only the interaction of particles and fibres with the matrix is important for such simulations, but also the mutual interaction of particles and fibres influences the behaviour of composite materials. Some TRBF's are given in Section 2 and some important applications and results are shown in Section 3. Discussion on some other types of TRBF's, applications and future research is contained in Section 4.

2. Some TRBF's

Let's consider linear elastic isotropic material with material constants G and ν being the shear modulus and Poisson's ratio, respectively.

Basic RBF will be the fundamental solution of the elasticity (Kelvin solution). The field of displacements in an elastic continuum by a unit force acting in direction of the axis x_p is given by the Kelvin solution

$$U_{pi}^{(F)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r}\left[(3-4\nu)\delta_{ip} + r_{,i}r_{,p}\right] \tag{1}$$

where x_i denotes the i-th coordinate of the displacement, r is the distance between the source point s, where the force is acting and a field point t, where the displacement is introduced, i.e.

$$r = \sqrt{r_i r_i}\,, \qquad r_i = x_i(t) - x_i(s). \tag{2}$$

The summation convention over repeated indices acts and

$$r_{,i} = \partial r/\partial x_i(t) = r_i/r \tag{3}$$

is the directional derivative of the radius vector r.

The gradients of displacement fields are corresponding derivatives of the field (1) in the point t,

$$U_{pi,j}^{(F)} = -\frac{1}{16\pi G(1-\nu)r^2}\left[(3-4\nu)\delta_{pi}r_{,j} - \delta_{pj}r_{,i} - \delta_{pj}r_{,p} + 3r_{,i}r_{,j}r_{,p}\right]. \tag{4}$$

Note that the second derivative of the radius vector of n-th power is

$$\left(r_{,k}^{n}\right)_{,j} = \frac{n}{r}\left(r_{,k}^{n-1}\delta_{jk} - r_{,j}r_{,k}^{n}\right). \tag{5}$$

The strains are

$$E_{pij}^{(F)} = \frac{1}{2}\left(U_{pi,j}^{(F)} + U_{pj,i}^{(F)}\right) = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^2}\left[(1-2\nu)(\delta_{pi}r_{,j} + \delta_{pj}r_{,i}) - \delta_{ij}r_{,p} + 3r_{,i}r_{,j}r_{,p}\right] \tag{6}$$

and the ij stress components of this field are

$$S_{pij}^{(F)} = 2GE_{pij}^{(F)} + \frac{2G\upsilon}{1-2\nu}\delta_{ij}E_{pkk}^{(F)} = \frac{1}{8\pi(1-\nu)}\frac{1}{r^2}\left[(1-2\nu)(\delta_{ij}r_{,p} - \delta_{jp}r_{,i} - \delta_{ip}r_{,j}) - 3r_{,i}r_{,j}r_{,p}\right] \tag{7}$$

where δ_{ij} is the Kronecker delta.

The next RBF's are obtained from derivatives of the fundamental solution. They will denote a dipole and a couple [1, 10]. The displacement field of a dipole can be obtained from the displacement field of a force by differentiating it in the direction of the acting force, i.e.

$$U_{pi}^{(D)} = U_{pi,p}^{(F)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^2}\left[3r_{,i}r_{,p}^2 - r_{,i} + 2(1-\nu)r_{,p}\delta_{ip}\right]. \tag{8}$$

The summation convention does not act over the repeated indices p here and in the following relations, too.

Gradients of the displacement field are

$$\begin{aligned} U_{pi,j}^{(D)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\big[&-15r_{,i}r_{,j}r_{,p}^2 + 3r_{,i}r_{,j} \\ &+ 2(1-2\nu)\delta_{ip}(\delta_{jp} - 3r_{,j}r_{,p}) + 6r_{,i}r_{,p}\delta_{jp} + \delta_{ip}(3r_{,p}^2 - 1)\big] \end{aligned} \tag{9}$$

and the corresponding strain and stress fields are

$$\begin{aligned} E_{pij}^{(D)} &= \frac{1}{2}\left(U_{pi,j}^{(D)} + U_{pj,i}^{(D)}\right) \\ &= -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\big[-15r_{,i}r_{,j}r_{,p}^2 + 3r_{,i}r_{,j} + 2(1-2\nu)\delta_{ip}\delta_{jp} \\ &\quad + 6\nu(\delta_{ip}r_{,j}r_{,p} + \delta_{jp}r_{,i}r_{,p}) + \delta_{ij}(3r_{,p}^2 - 1)\big], \end{aligned} \tag{10}$$

$$\begin{aligned} S_{pij}^{(D)} &= 2GE_{pij}^{(D)} + \frac{2G\upsilon}{1-2\nu}\delta_{ij}E_{pkk}^{(D)} \\ &= \frac{1}{8\pi(1-\nu)}\frac{1}{r^3}\big[(1-2\nu)(2\delta_{ip}\delta_{jp} + 3r_{,p}^2\delta_{ij} - \delta_{ij}) \\ &\quad + 6\nu r_{,p}(r_{,i}\delta_{jp} + r_{,j}\delta_{ip}) + 3(1-5r_{,p}^2)r_{,i}r_{,j}\big] \end{aligned} \tag{11}$$

The displacements (1) by a force are weak singular, the displacement gradients, strains and stresses are strong singular. The fields defined by a dipole have one order higher singularity (strong singularity in the displacement field and hyper-singularities in the strain and stress fields).

The derivatives in perpendicular direction to the force define the force couple [1, 10]. The displacement field for the couple is

$$U_{pi}^{(C)} = U_{pi,i}^{(F)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^2}\left[3r_{,p}r_{,i}^2 - r_{,p} + 2(1-\nu)r_{,i}\delta_{ip}\right] \tag{12}$$

and the corresponding strain and stress fields are

$$E_{pij}^{(C)} = \frac{1}{2}\left(U_{pi,j}^{(C)} + U_{pj,i}^{(C)}\right)$$
$$= -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\left[-15r_{,p}r_{,j}r_{,i}^2 + 3r_{,p}r_{,j} + 2(1-2\nu)\,\delta_{ip}\,\delta_{jp}\right.$$
$$\left. + 6\nu\left(\delta_{ip}r_{,i}r_{,j} + \delta_{ij}r_{,i}r_{,p}\right) + \delta_{jp}(3r_{,i}^2 - 1)\right], \tag{13}$$

$$S_{pij}^{(C)} = 2GE_{pij}^{(C)} + \frac{2Gv}{1-2\nu}\delta_{ij}E_{pkk}^{(C)}$$
$$= -\frac{1}{8\pi(1-\nu)}\frac{1}{r^3}\left[(1-2\nu)(2\delta_{ip}\delta_{ij} + 3r_{,i}^2\delta_{jp} - \delta_{jp})\right.$$
$$\left. + 6\nu r_{,i}(r_{,j}\delta_{ip} + r_{,p}\delta_{ij}) + 3(1-5r_{,i}^2)r_{,p}r_{,j}\right] \tag{14}$$

The RBF can be used also for simulation of the interaction between matrix and particles with very large aspect ratio such as composites reinforced with short fibres where the aspect ratio can be 1000:1 or even larger. The inter-domain boundary conditions can be simulated by 1D distribution of the TRBF's (source functions) along the fibre axis. When the TRBF's are approximated by polynomials then the problems lead to evaluation of following integrals

$$\int_a^b \frac{x_s^n (x_s - x_f)^p}{(y^2 + x_s - x_f^2)^{\frac{m}{2}+r}}\,\mathrm{d}x_s = f(x_f) \tag{15}$$

where x is the coordinate along the fibre axis, the subscripts s and f denote the source and field point and exponents are integer numbers and y is the distance of the field point from the source point. For computational purpose the integral (12) is transformed to

$$\int_{a+x_f}^{b+x_f} \frac{(x+x_f)^n\, x^p}{(y^2+x^2)^{\frac{m}{2}+r}}\,\mathrm{d}x = f(x_f). \tag{16}$$

The numerical integration of such integrals would be computationally very laborious because of the quasi-singularities and quasi-hyper-singularities in the integrals; however, analytic evaluation of the integrals containing the kernel function and polynomial approximation of the unknown function is very elegant way of numerical evaluation of the integrals, if the axis of the fibre is straight, i.e. the value of y is constant in the integrals above.

3. Some applications and results

Composite materials reinforced by stiff particles or fibres are important materials possessing excellent mechanical and also thermal and electro-magnetic properties. Understanding the behaviour of such composite materials is essential for structural design. Such composites contain huge number of reinforcing elements with large gradients in all fields in small parts of the matrix (in micro scale) around the reinforcing elements and accurate computational models are important for homogenization of material properties in macro scale (adjustment of local stiffness of such material) and for evaluation of strength of material. Micromechanics is essentially a multiscale theory: Although a "representative volume element" (RVE) can be viewed as a material point at the macro scale, it is associated with specific microstructure at the micro scale. It is well known that using volume element approximation such as FEM hundreds of elements are necessary to achieve required accuracy even for simple problem (see [3] where 50 000 to 100 000 trilinear elements were used for problem containing one spherical particle in the matrix).

The classical Eshelby solution [2] was obtained for an elastic isotropic inclusion in an infinite elastic matrix. The treatment of the RVE as an infinite space implies that the inclusion concentration is dilute, and therefore, a direct application of these results to the case of finite inclusion concentration is only approximate. An improved model was suggested by Mori and Tanaka [17]. Their method also assumes the absence of all inhomogeneities, but it includes certain effect of the inhomogeneity by taking average strain in the matrix phase when all inhomogeneities are present. Modification of existing homogenization methods via finite Eshelby tensors [22] provides significant improvement in predicting the behaviour of composites. In particular, the Hashin–Shtrikman variational bounds are modified according to the prescribed boundary condition [8, 22]. Recently, Li [25] solved the elastic field of an idealized, spherical, finite RVE embedded in an infinite, homogeneous, isotropic medium using Boundary Integral Equations (BIE). A solution is found which satisfies the continuity of displacements and traction fields across the RVE/composite interface. However, the model is simplified and does not take into account the interaction of discretely distributed particles in the matrix and calculates the Eshelby tensor from simplified Dirichlet and Neumann boundary conditions.

We do not aim to review papers using BEM, FEM and FMM concerning simulation of composite materials reinforced by particles and fibres. The number of published papers is not large, but it is increasing. Some representative results using Fast Multipole BEM (FMBEM) are published in [15, 19, 24].

If the ideas of the TRBF and MFS are used then simple and efficient formulation can be developed. In the case of composite material reinforced by spheres or particles with aspect ratio not very different from 1, a particle can be modeled by a triple dipole located in the centre of the particle and the intensities of the dipole can be computed by using small number of collocation points on the particle boundary (see Fig. 1). The method of discrete dipoles is very simple and details can be found in [14].

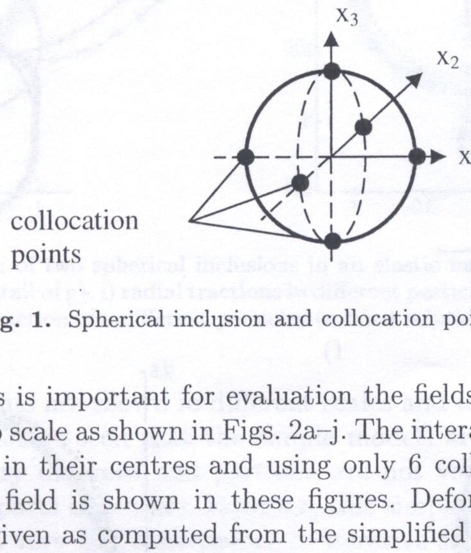

Fig. 1. Spherical inclusion and collocation points

The interaction of particles is important for evaluation the fields in the microstructure and for reinforcing effects in the macro scale as shown in Figs. 2a–j. The interaction of two particles modelled by two triple dipoles located in their centres and using only 6 collocation points on the particle boundaries in an eigenstrain field is shown in these figures. Deformation, radial and tangential components of tractions are given as computed from the simplified models for two different cases: 1) particles with equal size radii and with distance between the particles same size as their radius and 2) radius of smaller particle equal to one fifth of the radius of larger one and with the distance between particles equal to one fifth of the radius of the smaller particle. In the last case also the local parts of deformation and tangential tractions in the vicinity of another particle are shown. As boundary conditions the difference of displacements in direction of the vector connecting two points at opposite sides of the particle are prescribed for eigenstrain state of the particle. In this way, it is not necessary to keep for rigid body displacement of particles and also the equilibrium is automatically satisfied as a dipole is in static equilibrium. All fields are split to the eigenstrain and local parts. The undeformed form of particles is denoted by dots, and corresponding deformation and traction fields are given by circles. Intensity of tractions is given by radial distance of corresponding circle from the undeformed form. Recall that for the deformed form of spherical particle in the eigenstrain [22, 25], only the local parts of deformation and tractions are shown in the figures, i.e. if the particle is rigid the local deformation of sphere should follow the dotted lines in corresponding

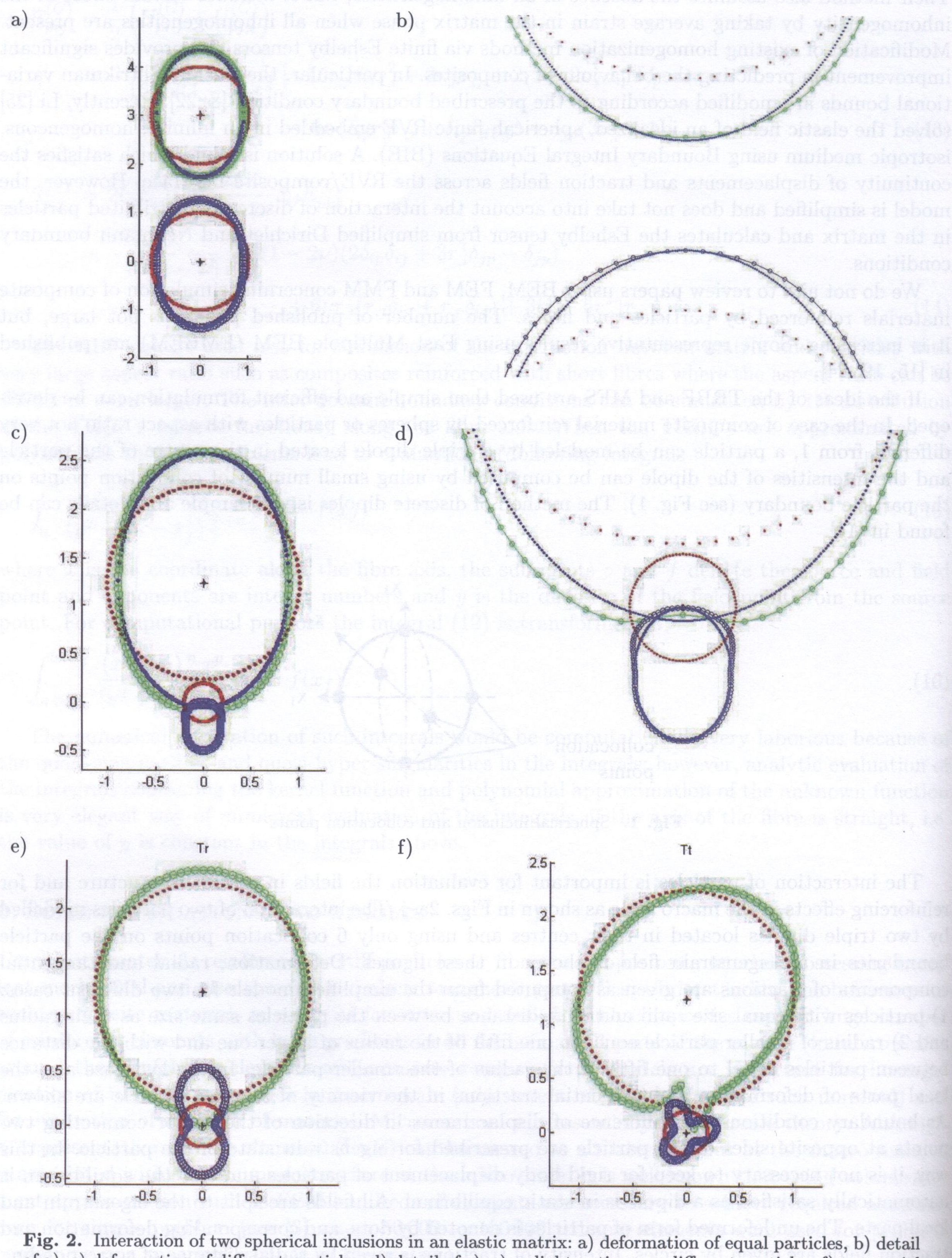

Fig. 2. Interaction of two spherical inclusions in an elastic matrix: a) deformation of equal particles, b) detail of a), c) deformation of different particles, d) detail of c), e) radial tractions on different particles, f) tangential tractions on different particles *(continued on the next page)*

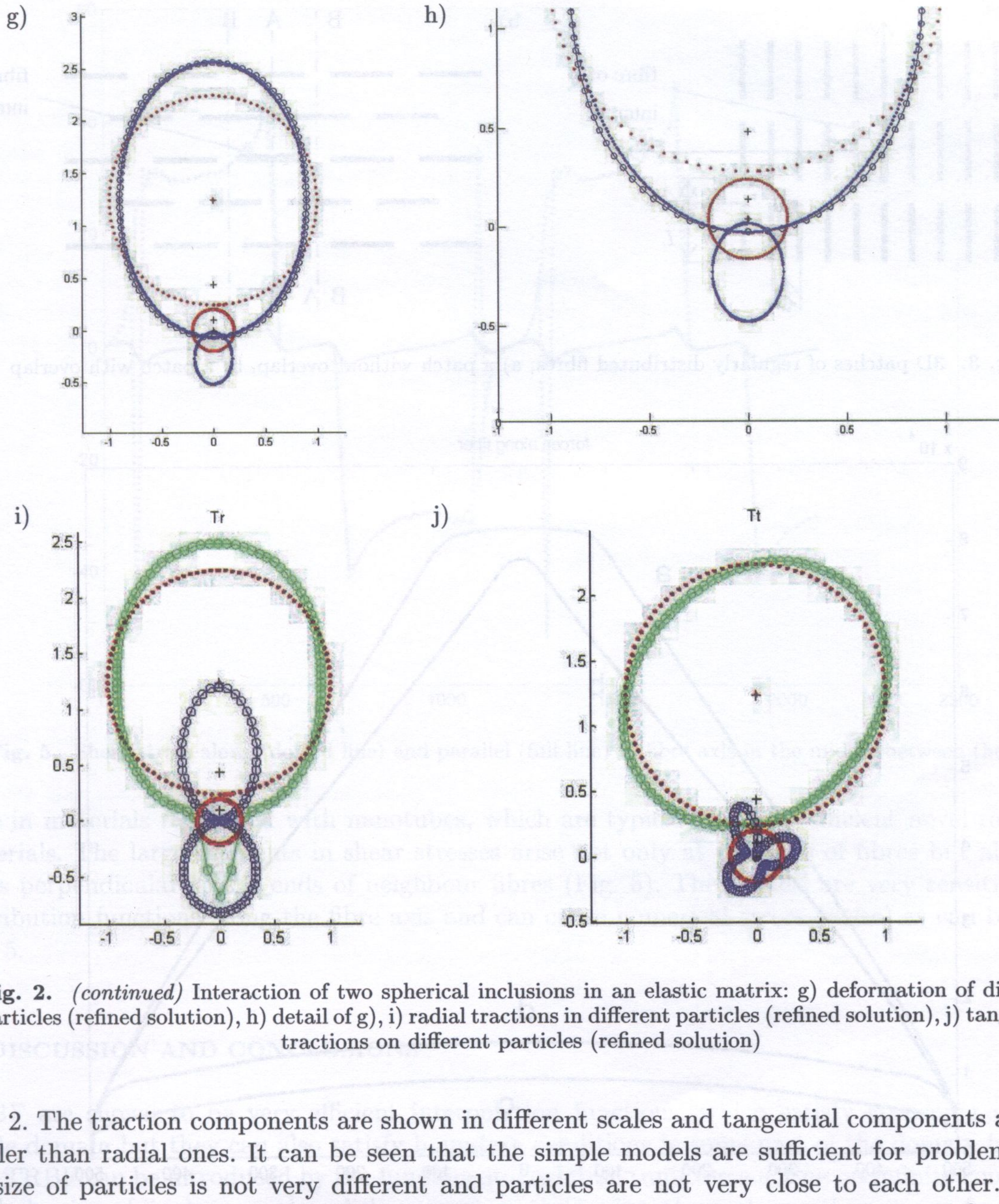

Fig. 2. *(continued)* Interaction of two spherical inclusions in an elastic matrix: g) deformation of different particles (refined solution), h) detail of g), i) radial tractions in different particles (refined solution), j) tangential tractions on different particles (refined solution)

Figs. 2. The traction components are shown in different scales and tangential components are much smaller than radial ones. It can be seen that the simple models are sufficient for problems, when the size of particles is not very different and particles are not very close to each other. Refined models are required for small parts of models. However, this simple model can be used for iterative improvements of solution with very fast convergence in iterative steps for each, very stiff or elastic inclusions. Additional interpolation functions are included in the iterative steps.

Much more complicated interaction is in material reinforced by fibres. The interaction can be followed in patches of regularly distributed straight fibres with and without overlap (Fig. 3) in direction perpendicular to the fibre axes. method of discrete dipoles is very simple and details can be found in [14].

As the fibres are long and thin, they are much stiffer in axial direction than in bending and the satisfaction of continuity of displacements, strains and tractions on the surface between the matrix and fibres and corresponding displacements and strains along the fibre would require a very large number of TRBF (source points) to simulate the interaction.

Moreover, in the end parts of a fibre the fields have very large gradients, which increases the difficulties with accuracy and numerical stability of the solution. In our models, continuous distribution of source points is used for simulation of the interaction. It is possible to use both distributed forces and distributed dipoles along the fibre axis (1D distribution) and oriented in the axis direction

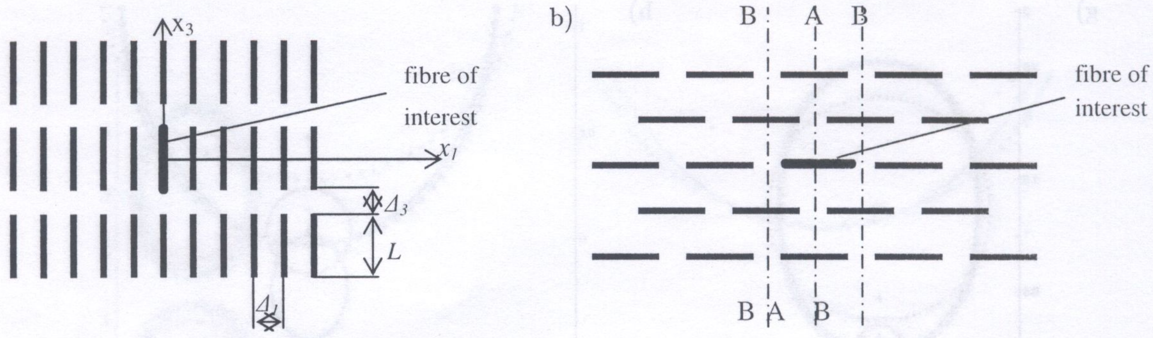

Fig. 3. 3D patches of regularly distributed fibres; a) a patch without overlap, b) a patch with overlap

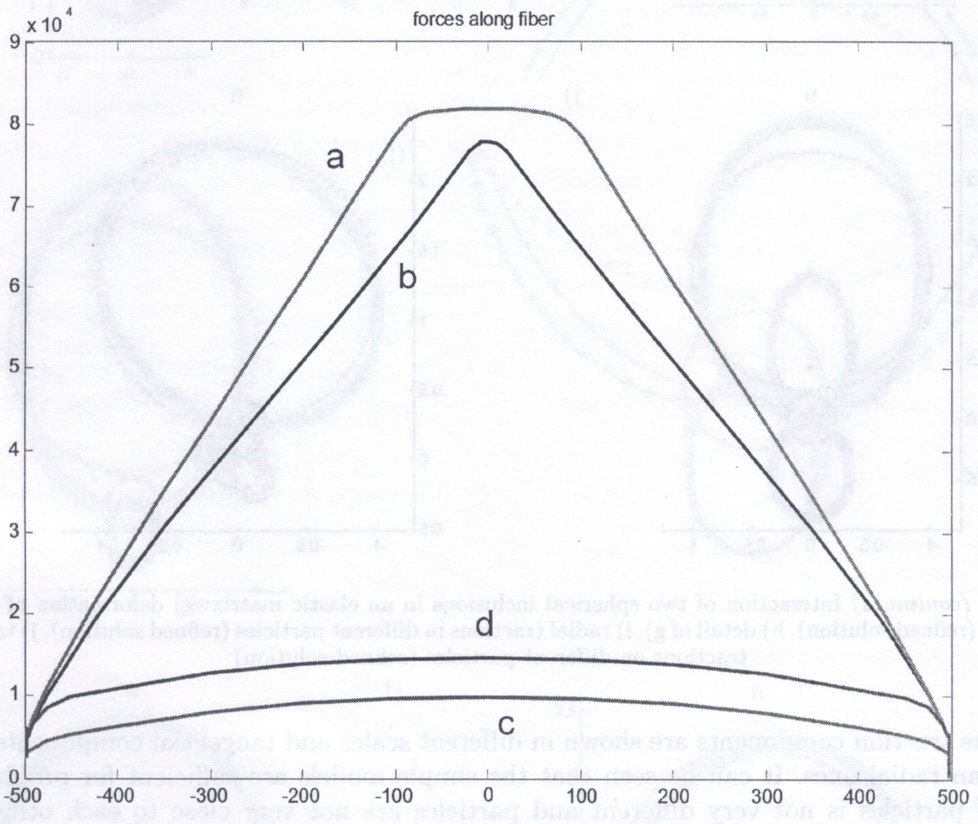

Fig. 4. Forces in fibre cross section with overlap, 'a' and 'b' black, and without overlap, 'c' and 'd', by different gap between fibres in longitudinal direction

in the model. Their role is mainly to satisfy continuity in the fibre axis direction. Continuity in directions perpendicular to the fibre axis is served mainly by the continuous dipoles along the fibre axis, but directed perpendicularly to the fibre axis. Recall that continuously distributed dipoles are derivatives of continuously distributed forces. The distribution is approximated by piecewise quadratic functions with C^0 continuity between the elements. More about the model can be found in [12].

The forces in the fibres are much greater if the fibres overlap than in the fibres without the overlap (Fig. 4) and thus the stiffening effect is considerably influenced by the overlapping. The forces can lead to axial stresses which can exceed the stresses in the matrix by several orders and can cause fracture of the fibres in tension or loss of stability in compression.

Extreme shear forces between the fibre and the matrix can lead to de-bonding of the fibre or to de-cohesion and re-cohesion at the ends and also in the middle of a fibre close to another

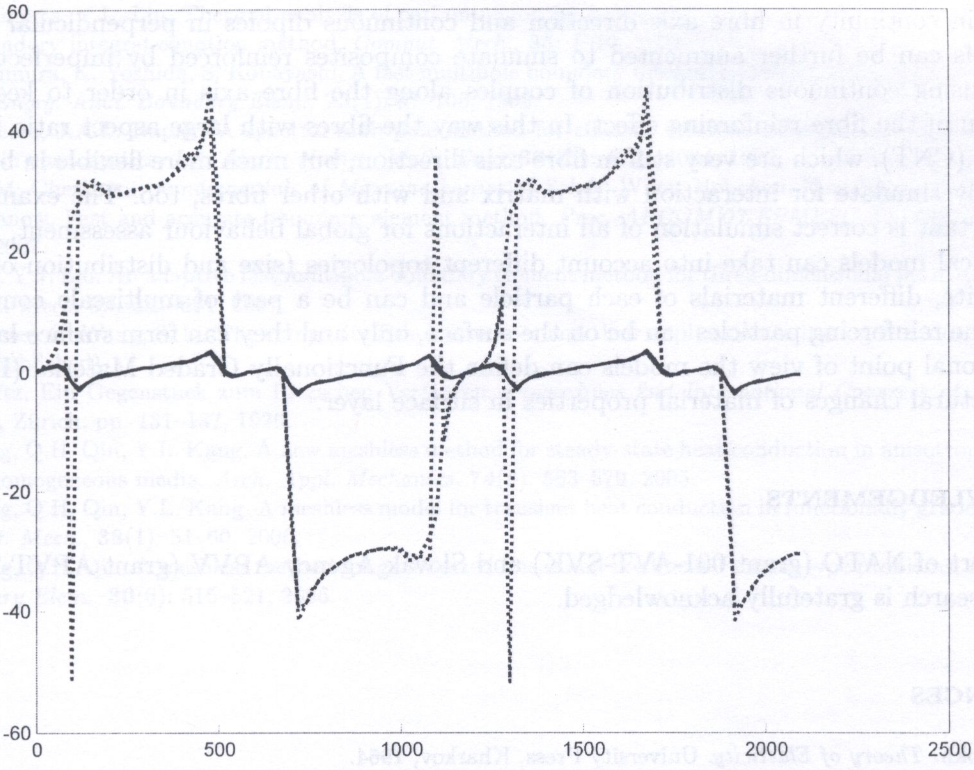

Fig. 5. Shear stress along (dotted line) and parallel (full line) to fibre axis in the middle between the fibres

fibre in materials reinforced with nanotubes, which are typical and very efficient novel reinforcing materials. The large gradients in shear stresses arise not only at the ends of fibres but also in the parts perpendicular to the ends of neighbour fibres (Fig. 5). The models are very sensitive to 1D distribution functions along the fibre axis and can cause numerical errors (noise) as can be seen in Fig. 5.

4. Discussion and conclusions

TRBF are shown to be very efficient interpolation functions, which satisfy governing equations inside domain but they can also satisfy boundary conditions in some part of the domain boundary. The TRBF can be introduced by the fundamental solution (unit force acting on infinite continuum), its derivatives (dipoles, couples, dislocations) in mechanics, thermal, or other source functions in other field problems. The TRBF correctly simulate decaying of field variables and so, they can efficiently model any concentrators in field variables. They can be also source functions acting in other domains (Boussinesq–Cerutti solution for half space which can be used for effective modeling of effect of local loading [12], analytic solution for layered structures, etc.).

It is demonstrated that the TRBF's can be used in connection with boundary collocation methods to simulate a microstructure reinforced by particles using ideas similar to MFS with only single triple dipoles located into centres of the particles to simulate the interaction of particles with matrix and with other particles, as well. No mashing and no integration are necessary. The ideas of FMM are also possible to formulate using mechanical principles instead of Taylor series expansions by the formulations. The far field interaction is then introduced by resulting dipole taking into account force and moment equilibrium.

For simulation of a microstructure reinforced with short fibres 1D continuous distribution (it is the TRBF, too) of source functions were developed by authors. It can reduce the model comparing to other numerical models by many orders. The forces or dipoles can be used for simulation of interdomain continuity in fibre axis direction and continuous dipoles in perpendicular directions. The models can be further augmented to simulate composites reinforced by imperfect or curved fibres by using continuous distribution of couples along the fibre axis in order to keep moment equilibrium of the fibre reinforcing effect. In this way the fibres with large aspect ratio like carbon nanotubes (CNT), which are very stiff in fibre axis direction, but much more flexible in bending can be correctly simulate for interaction with matrix and with other fibres, too. The examples show, how important is correct simulation of all interactions for global behaviour assessment.

Numerical models can take into account different topologies (size and distribution of particles) of composite, different materials of each particle and can be a part of multiscale computational models. The reinforcing particles can be on the surface, only and they can form surface layers. From computational point of view the models can define the Functionally Graded Material (FGM) from microstructural changes of material properties in surface layer.

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