FINAL SCIENTIFC/TECHNICAL REPORT

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Project Title: Numerical Stochastic Homogenization Method and Multiscale Stochastic Finite Element Method – A Paradigm for Multiscale Computation of Stochastic PDEs

Principle Investigator: X. Frank Xu

2. Authorized Distribution Limitation Notices: None

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3. Executive Summary

Multiscale modeling of stochastic systems, or uncertainty quantization of multiscale modeling is becoming an emerging research frontier, with rapidly growing engineering applications in nanotechnology, biotechnology, advanced materials, and geo-systems, etc. While tremendous efforts have been devoted to either stochastic methods or multiscale methods, little combined work had been done on integration of multiscale and stochastic methods, and there was no method formally available to tackle multiscale problems involving uncertainties. By developing an innovative Multiscale Stochastic Finite Element Method (MSFEM), this research has made a ground-breaking contribution to the emerging field of Multiscale Stochastic Modeling (MSM) (Fig 1). The theory of MSFEM basically decomposes a boundary value problem of random microstructure into a slow scale deterministic problem and a fast scale stochastic one. The slow scale problem corresponds to common engineering modeling practices where fine-scale microstructure is approximated by certain effective constitutive constants, which can be solved by using standard numerical solvers. The fast scale problem evaluates fluctuations of local quantities due to random microstructure, which is important for scale-coupling systems and particularly those involving failure mechanisms. The Green-function-based fast-scale solver developed in this research overcomes the curse-of-dimensionality commonly met in conventional approaches, by proposing a random field-based orthogonal expansion approach. The MSFEM formulated in this project paves the way to deliver the first computational tool/software on uncertainty quantification of multiscale systems. The applications of MSFEM on engineering problems will directly enhance our modeling capability on materials science (composite materials, nanostructures), geophysics (porous media, earthquake), biological systems (biological tissues, bones, protein folding). Continuous development of MSFEM will further contribute to the establishment of Multiscale Stochastic Modeling strategy, and thereby potentially to bring paradigm-shifting changes to simulation and modeling of complex systems cutting across multidisciplinary fields.

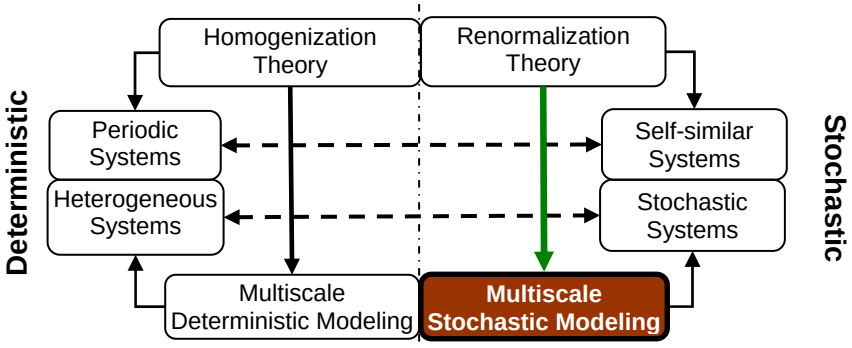

Figure 1: Parallel paths of Homogenization-MDM & Renormalization–MSM (Xu et al, 2009)

4. A comparison of the actual accomplishments with the goals and objectives

4.1 Objectives quoted from the project proposal

"By developing formulation and algorithms, this research will provide to scientific and engineering communities novel computational methods for multiscale stochastic elliptic partial differential equations (PDEs). Two multiscale stochastic numerical methods, the numerical stochastic homogenization method (NSHM) and the multiscale stochastic finite element method (MsSFEM), will be formally established to solve stochastic boundary value problems characterized with highly oscillating stationary and non-stationary random coefficients, respectively. The three-year research program will accomplish the development stage of multiscale stochastic numerical methods for stochastic boundary value problems, based on which software production and solvers for realistic problems will become attainable in the future production stage (Figure 4.5). The methods developed in this research program are further expected to act as a paradigm for solving of general stochastic PDEs involving multiscale stochastic data."

4.2 Actual accomplishments

1. The numerical stochastic homogenization method has been formally established with formulation of stochastic variational principles (Xu, 2009) and numerical implementation on multi-phase heterogeneous materials (Xu and Chen, 2009);
2. Based on a preliminary multiscale stochastic framework on elliptic PDEs (Xu, 2007), MSFEM has been formally established for elastic boundary value problems of both stationary and non-stationary random heterogeneous materials (Xu et al, 2009). Various numerical algorithms to implement MSFEM have been developed (Shen and Xu, 2010).

The MSFEM formulated has become ready for the next stage of software production, and the primary goals of the project have been completely achieved. In the addition to the above accomplishments, the following works related to multiscale stochastic modeling of materials have been performed under the sponsorship of this project:

3. Multiscale stochastic modeling of strength of nanocomposites (Xu et al, 2010; Beyerlein et al, 2009);
4. Stochastic modeling of fracture of random materials (Yang and Xu, 2008; Hu and Xu, 2009).

5. Summary of Project Activities

5.1 Original hypotheses and underlying variational principles

An elastic boundary value problem (BVP) of random heterogeneous materials is governed by a 4^{th}-order elliptic equation with randomly fluctuating coefficients (elastic

moduli) represented by a multi-phase random field. Since the focus of this research is on uncertainty quantification of responses due to spatial randomness of microstructures, the body force and boundary conditions are assumed to be deterministic.

To develop a finite element computational model for multiscale stochastic boundary value problems, the underlying stochastic variational principles are required, analogous to the role played by deterministic variational principles in the classical finite element formulation. In (Xu, 2009) two new stochastic variational principles are formulated, which provide a theoretical foundation for formulation of MSFEM.

5.2 Approaches used

For scale-decoupling problems when there is a clear scale separation between the size of a BVP and the size of microstructure, the stochastic homogenization approach can be applied to solving of multiscale problems involving uncertainties. To quantify the scale-coupling effects, or assess the minimal size of representative volume element, a numerical stochastic homogenization method is developed in (Xu and Chen, 2009).

For scale-coupling problems occurring in small-scale systems such as NEMS/MEMS, and failure problems, classical homogenization approach is inapplicable, and MSFEM is developed in this project. The underlying theory of the MSFEM is the stochastic variational principles formulated in (Xu, 2009). By decomposing a random BVP into a slow-scale BVP and fast-scale one, the original PDE is transformed into an integral equation and Green-function-based finite element method is therefore developed to resolve the equation. More description of the computer model is given in Section 7 of this report.

5.3 Problems encountered and departure from planned methodology and assessment of the impacts on the project results

The MSFEM formulated in this project has been applied onto random heterogeneous materials characterized with stationary random fields. For non-stationary problems as originally planned, although the formulation of the MSFEM is identically applicable, the computational algorithms need to be modified and improved, especially for nonlinear problems characterized with evolving non-stationary random fields. The continuous efforts along this direction are underway (with proposals to NSF pending), and the breakthrough is expected to significantly enhance predictive capability of failure of materials.

5.4 Facts, figures, analyses and assumption used to support the conclusions

The underlying theory of the MSFEM is rigorously derived as the stochastic variational principles for stochastic BVP (Xu, 2009). The facts, figures, and assumption about the verification and numerical accuracy of MSFEM are provided in Section 7 specifically.

6. Products Developed Under the Award

6. 1 Publications

Peer Reviewed Journal Articles

1. X.F. Xu, K Hu, I.J. Beyerlein, and G. Deodatis, "Statistical strength of hierarchical carbon nanotube composites", to be submitted
2. L. Shen and X.F. Xu, "Multiscale Stochastic Finite Element Modeling of Random Elastic Heterogeneous Materials", Computational Mechanics, 2010, 45 (6) 607-621
3. I.J. Beyerlein, P.K. Porwal, Y.T. Zhu, K. Hu and X.F. Xu, "Scale and twist effects on the strength of nanostructured yarns and reinforced composites", Nanotechnology, 2009, 20, 485702
4. X.F. Xu, X. Chen, and L. Shen, "A Green-Function-Based Multiscale Method for Uncertainty Quantification of Finite Body Random Heterogeneous Materials", Computers and Structures, 2009, 87, 1416-1426
5. K. Hu and X.F. Xu, "Probabilistic Upscaling of Material Failure Using Random Field Models - A Preliminary Investigation", Algorithms (special issue on Numerical Simulation of Discontinuities in Mechanics) , 2009, 2(2), 750-763
6. X.F. Xu, "Generalized Variational Principles for Uncertainty Quantification of Boundary Value Problems of Random Heterogeneous Materials", ASCE Journal of Engineering Mechanics, 2009, 135 (10) 1180-1188
7. X.F. Xu and X. Chen, "Stochastic Homogenization of Random Multi-phase Composites and Size Quantification of Representative Volume Element", Mechanics of Materials (2009) 41 (2) 174-186
8. Z.J. Yang and X.F. Xu, "A Heterogeneous Cohesive Model for Quasi-Brittle Materials Considering Spatially Varying Random Fracture Properties", Comput. Methods Appl. Mech. Engrg. (2008) 197 (45-48) 4027-4039
9. X.F. Xu, "A multiscale stochastic finite element method on elliptic problems involving uncertainties", Comput. Methods Appl. Mech. Engrg. (2007) 196 (25-28) 2723-2736

Book Chapter

10. I.J. Beyerlein, P.K. Porwal, Y.T. Zhu, X.F. Xu, S.L. Phoenix, "Probabilistic strength of carbon nanotube yarns", Advances in Mathematical Modeling and Experimental Methods for Materials and Structures: The Jacob Aboudi Volume. Gilat and Banks-Sills, (eds.), Springer. 2010

Proceedings

11. X.F. Xu, "Multiscale Modeling of Random Heterogeneous Materials", Proceedings of the 10th International Conference on Structural Safety and Reliability, Osaka, Japan, September 13~17, 2009
12. L. Shen and X.F. Xu, "Multiscale Stochastic Finite Element Method on Random Boundary Value Problems", The second International Conference on High

Performance Computing and Applications, Lecture Notes in Computer Science, Springer, August 10~12, 2009
13. X.F. Xu, "A Random-Field Based Orthogonal Expansion Method to Circumvent Curse-of-Dimension in Multiscale Modeling of Random Media Problems", Proceedings of the Fourth Biot Conference on Poromechanics, Columbia University, New York City, June 8~10, 2009
14. Z.J. Yang and X.F. Xu, "Modelling cohesive crack propagation in concrete considering random heterogeneous fracture properties", Proceedings of the 9th Int Conf Computational Structures Technology. Athens, Greece, CD (paper No. 245), Sept 2008,
15. K. Hu, X.F. Xu, "A reliability-based hierarchical multiscale model for failure prediction", Proceedings of the Inaugural International Conference of the Engineering Mechanics Institute, Minneapolis, MN, May 18~21, 2008
16. X. Chen, and X.F. Xu, "Uncertainty quantification of boundary value problems of random materials", Proceedings of the Inaugural International Conference of the Engineering Mechanics Institute, Minneapolis, MN, May 18~21, 2008
17. X.F. Xu, I.J. Beyerlein, K. Hu, G. Deodatis, "Multiscale stochastic modeling of the failure of fiber reinforced composites", Proceedings of the 49th AIAA/ASME/ASCE/AHS/ ASC Structures, Structural Dynamics, and Materials Conference, Schaumburg, Illinois, April 7~10, 2008; AIAA-2008-2292
18. X.F. Xu and Keqiang Hu, "Size effect of stochastic representative volume element on multiscale damage modeling", Proceedings of the 18th ASCE Engineering Mechanics Conference, Blackburg, VA, 2007

6.2 Networks or collaborations fostered

- Professor Manolis Papadrakakis (National technical University of Athens, Greece) and Dr. George Stefanou (National technical University of Athens, Greece) on multiscale stochastic modeling techniques;
- Professor Aihui Zhou (Chinese Academy of Sciences) and Dr Lihua Shen (Capital Normal University, China) on numerical algorithms of MSFEM;
- Professor George Deodatis (Columbia University) and Dr. Irene Beyerlein (Las Alamos National Laboratory) on multiscale stochastic modeling of nanocomposites;
- Dr. Zhenjun Yang (University of Liverpool) on stochastic modeling of fracture;
- Dr. Xi Chen (Beijing Jiaotong University) MSFEM on geotechnical engineering.

6.3 Software

Two MSFEM computing codes have been developed using Matlab and C++, respectively.

7. Information Involving Computer Modeling

7.1 Model description, key assumption, version, source and intended use

Model description Based on the stochastic variational principles proposed in (Xu, 2009), a Green-function-based (GFB) multiscale method is formulated in (Xu et al, 2009; Shen and Xu, 2010) to decompose a BVP of random microstructure into a slow scale deterministic problem and a fast scale stochastic one (Fig. 2), with the flow chart shown in Fig 2. The slow scale problem corresponds to common engineering modeling practices where fine-scale microstructure is ignored by choosing appropriate effective constitutive constants. The fast scale problem evaluates fluctuations of local quantities due to random microstructure, which is important for scale-coupling systems and particularly those involving failure mechanisms. To resolve the fast scale problem, a novel GFB finite element method is developed which is numerically efficient to capture effects of local microstructure.

Key assumption Both body force and boundary conditions are assumed to be deterministic. The two-point/second-order correlation function used in the model is assumed to be known, and in the examples an exponential function is used.

Version The primary version of MSFEM is developed for linear problems (elasticity). The future version of MSFEM will include the extension to nonlinear problems (e.g. plasticity, damage and fracture) which is under ongoing development.

Source Two MSFEM computing codes have been developed using Matlab and C++, respectively.

Intended use The current version of MSFEM is developed for uncertainty quantification of stress and strain due to randomness or incompleteness of microstructural information, provided the second-order correlation function is given.

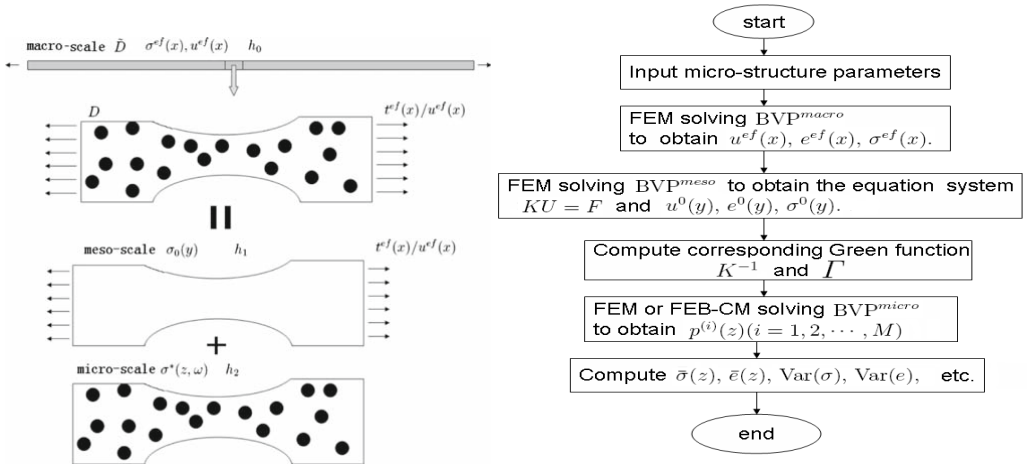

Fig 2. Left) A meso-scale BVP is decomposed into a slow scale problem and a fast/micro-scale one; Right) Flow chart of MSFEM (Shen & Xu, 2010)

7.2 Performance criteria for the model related to the intended use

The current MSFEM version is verified by comparison with the available theoretical solutions for special cases of stochastic boundary value problems whereas the correlation length approaches zero or infinitely large. The efficiency of algorithms is evaluated by comparing the convergence rate with that of classical displacement-based finite elements.

7.3 Test results to demonstrate the model performance criteria were met

As shown in Fig 3, when the correlation length l_c =100 is significantly larger than the BVP size (10x10), the MSFEM solution converges to the theoretical solution for the special case with an infinitely large correlation length.

As shown in Table 1,2 &3 the error estimates vs. mesh size, the convergence rate of the Green-function-based FEM is of the order $O(h^2)$ for bilinear elements, which is one order faster than the classical displacement-based finite element method. The error estimates also indicate that the convergence rate becomes faster when the ratio between a correlation length and the BVP size is larger.

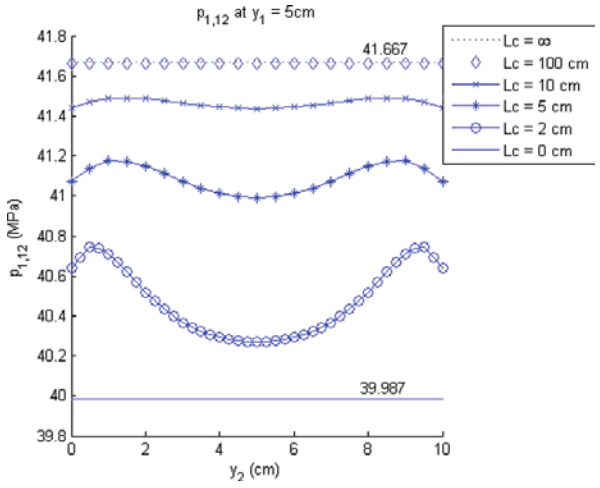

Fig 3. MSFEM solutions for a variety of correlation lengths (the dash and bottom lines corresponding to theoretical solutions) (Xu et al, 2009)

$h=h_1=h_2$	$\frac{\left\|p^h_{1,11}-p^*_{1,11}\right\|_{0,D}}{\left\|p^*_{1,11}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,22}-p^*_{1,22}\right\|_{0,D}}{\left\|p^*_{1,22}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,12}-p^*_{1,12}\right\|_{0,D}}{\left\|p^*_{1,12}\right\|_{0,D}}$
2cm (5x5)	1.802524e-001	1.802524e-001	3.825081e-004
1 cm (10x10)	7.289119e-002	7.289119e-002	1.109418e-004

Table 1: The errors of the solutions for l_c = 10 cm

$h=h_1=h_2$	$\frac{\left\|p^h_{1,11}-p^*_{1,11}\right\|_{0,D}}{\left\|p^*_{1,11}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,22}-p^*_{1,22}\right\|_{0,D}}{\left\|p^*_{1,22}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,12}-p^*_{1,12}\right\|_{0,D}}{\left\|p^*_{1,12}\right\|_{0,D}}$
2cm (5x5)	1.956638e-001	1.956638e-001	1.406193e-003
1 cm (10x10)	8.059657e-002	8.059657e-002	4.059999e-004
0.5 cm (20x20)	3.081771e-002	3.081771e-002	1.168850e-004

Table 2: The errors of the solutions for l_c = 5 cm

$h=h_1=h_2$	$\frac{\left\|p^h_{1,11}-p^*_{1,11}\right\|_{0,D}}{\left\|p^*_{1,11}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,22}-p^*_{1,22}\right\|_{0,D}}{\left\|p^*_{1,22}\right\|_{0,D}}$	$\frac{\left\|p^h_{1,12}-p^*_{1,12}\right\|_{0,D}}{\left\|p^*_{1,12}\right\|_{0,D}}$
2cm (5x5)	3.240674e-001	3.240674e-001	7.772499e-003
1 cm (10x10)	1.582296e-001	1.582296e-001	2.119706e-003
0.5 cm (20x20)	6.528419e-002	6.528419e-002	4.839603e-004

Table 3: The errors of the solutions for l_c = 2 cm

7.4 Theory behind the model

Over the past half century tremendous progress has been achieved in theoretical and computational mechanics, and scale-decoupling deterministic mechanics has been well established. Based on a fundamental assumption of macro-micro scale decoupling, micromechanics was first initiated around fifty years ago to investigate effects of microscopic heterogeneity and randomness on macroscopic behaviors. Major efforts have since been focused on evaluation of effective mechanical properties and variational bounds by incorporating statistical information of microstructures. While recent examination of the subject indicates a certain level of maturity on scale-decoupling micromechanics, the area of scale-coupling mechanics emerges on the horizon that addresses heterogeneity and randomness of materials across multiple length and time scales, particularly for the emerging high strength composite metamaterials.

A scale-coupling mechanics problem refers to a boundary value problem with one or more of its dimensions comparable to the characteristic length of heterogeneity, e.g., the thickness dimension of thin films and certain components of micro-electronic-mechanical systems (MEMS) being comparable to the grain size of polycrystals; or in failure phenomena when local statistical heterogeneity become crucial due to high sensitivity of local instabilities. For these cases, the classical scale-decoupling homogenization approach becomes inapplicable. A prevalent issue in computational mechanics is while a fine mesh is desired for achieving high accuracy, a certain mesh size threshold exists below which material properties of the finite elements become non-deterministic due to scale coupling effects between boundaries and heterogeneity inside elements, i.e. scale-decoupling deterministic finite elements become questionable. To tackle scale-coupling problems involving uncertainties and the curse-of-dimensionality,

novel multiscale methods and algorithms are required. Based on a stochastic variational formulation, a multiscale stochastic finite element method was recently proposed (Xu, 2007) to tackle multiscale elliptic problems involving uncertainties. It has been recognized that, to bring multiscale methods closer to real materials, new theories for scale-coupling mechanics and uncertainty quantification are demanded. One particularly notes that there are no rigorous variational principles available with respect to uncertainty quantification of boundary value problems. This forms a major motivation of this study.

Based on classical variational principles, generalized variational principles are presented in (Xu, 2009) for BVPs of random heterogeneous solids. It is worthnoting that classical variational principles are only useful for estimates of effective properties, e.g., elastic moduli of finite elements provided the element size is sufficiently larger than the size of heterogeneity, and are inapplicable for BVPs subjected to general boundary conditions. A complete picture of scale-coupling variational mechanics is presented in (Xu, 2009) which not only rigorously provides both deterministic and stochastic versions of generalized Hashin-Shtrikman and generalized energy principles, but critically formulates the boundary constraints to be satisfied by the Green's function and the stress polarization. By first developing a decomposition scheme for stochastic BVPs, both deterministic and stochastic versions of generalized variational principles are formulated, which provide upper and lower variational bounds to quantify the uncertainty of responses due to randomness or incompletes of microstructural information. The details of the principles refer to (Xu, 2009).

7.5 Mathematics to be used, including formulas and calculation methods

Based on the stochastic variational principles formulated, a random BVP is decomposed into a slow-scale deterministic BVP and fast-scale stochastic BVP. Since the slow-scale BVP can be solved by using standard finite elements, the model is reduced to that for a fast-scale BVP, while the formula for the latter is written as a Fredholm integral equation of the second kind involving the singular kernel

$$\Delta \mathbf{L}_s^{-1}\mathbf{p}_s(\mathbf{y})c_s + \sum_{r=1}^{M}\int_D \mathbf{\Gamma}(\mathbf{y},\mathbf{y}')c_{rs}(\mathbf{y}',\mathbf{y})\mathbf{p}_r(\mathbf{y}')d\mathbf{y}' = \mathbf{e}_0(\varepsilon\mathbf{y})c_s \qquad s = 1,2,...,M \qquad (1)$$

To resolve the above equation, three calculation methods have been developed (Xu, et al, 2009), i.e. Galerkin finite element method, the FE-based collocation method, and an iterative pseudo-spectral method. The numerical experiments on higher/linear order finite elements and collocation method demonstrate that

- The GFB finite element solution of the fast-scale BVP mostly depends on the accuracy of Green function approximation, and to compute Green function efficiently and accurately, higher order finite elements are better than linear ones, as shown in Fig. 4 Left).
- Convergence rate of Gelerkin finite element (weak) method is faster than finite element based collocation (strong) method, as shown in Fig 4 Right). With higher-order elements such as Hermite bicubic element, the FEB-CM can be much improved without the effect due to discontinuity of function, which remains for future investigation;

- The Green-function-based finite elements involve the singular kernel function. Use of triangular elements can lead to oscillating results with mesh sensitivity. Quadrilateral elements can generally avoid such undesired effect.

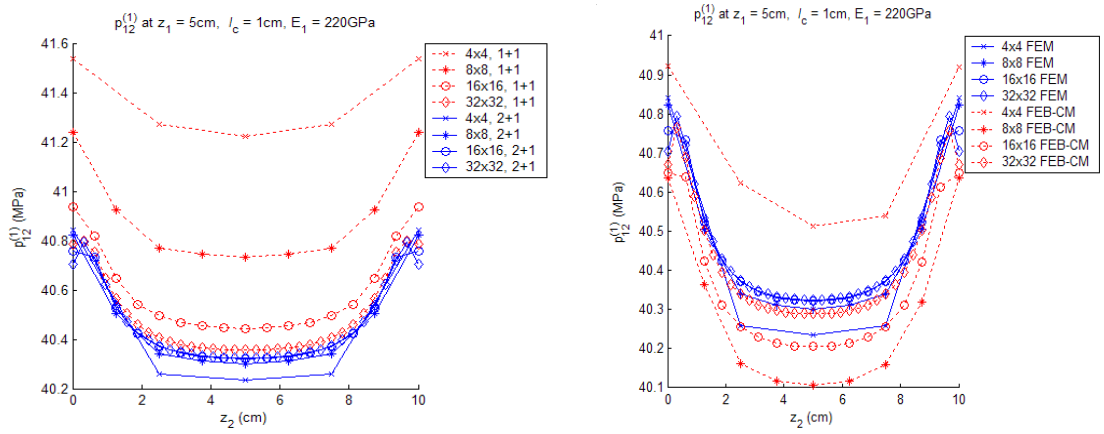

Fig 4. Left) Comparison of solution accuracy between linear (1+1) and quadratic elements; Right) Comparison between finite elements and collocation method

7.6 Whether or not the theory and mathematical algorithms were peer reviewed

The underlying scale-coupling theory in the context of formulated variational principles was peer reviewed and published in the Journal of Engineering Mechanics. The mathematical algorithms were peer reviewed and published in Journal of Computer and Structures and Computational Mechanics.

7.7 Hardware requirement

For a benchmark problem involving thousands of finite elements, currently a PC is sufficient to perform MSFEM computation. When tens of thousands or more elements are involved, or for nonlinear MSFEM computation, high performance hardware such as workstation is in need.

7.8 Documentation - Model Code

A MATLAB code for resolving elasticity of the fast-scale BVP is attached as part of this final report (the algorithmic part to obtain the slow-scale input, quadrature integration, and meshing are omitted).

```
%======================
% fsbvp3 – a fast-scale solver – March 30, 2010
% Developed & Written by Dr Xi Frank Xu,Stevens Institute of Technology
% Under the sponsorship of US Department of Energy
%======================

   clear
   t0=cputime;
   load G G;% Green function
   G=sparse(G);
   load EPXX EPXX % slow-scale strain
   load EPYY EPYY % slow-scale strain
   load EPXY EPXY % slow-scale strain

   c1=0.5;% volume fraction
   Lc=1; % correlation length
   E=200;MU=.2; % elastic moduli

%-------------------------
%  LOAD DATA
%-------------------------
   load MESHo   -ASCII
   load NODES   -ASCII
   load NP      -ASCII

   NUMNP = MESHo(1);
   NUMEL = MESHo(2);
   NNPE  = MESHo(3);

   XORD=NODES(:,1)';
```

```
   YORD=NODES(:,2)';
   NPcode=NODES(:,3)';

%  ----------------------
%  Declare sparse matrix
%  ----------------------

   K2 = zeros(NUMNP,NUMNP);
   K11 = zeros(NUMNP,NUMNP);
   K14 = zeros(NUMNP,NUMNP);
   K12 = zeros(NUMNP,NUMNP);
   K22 = zeros(NUMNP,NUMNP);
   K24 = zeros(NUMNP,NUMNP);
   K44 = zeros(NUMNP,NUMNP);

%  ----------------------
%  General Initialization
%  ----------------------
      if NNPE == 3
      NSPE=3;
      NNPS=2;
   elseif NNPE == 6
      NSPE=3;
      NNPS=3;
   elseif NNPE == 4
      NSPE=4;
      NNPS=2;
   elseif NNPE == 8
      NSPE=4;
      NNPS=3;
   end

   RHS1(1:NUMNP,1)=0;
   RHS2(1:NUMNP,1)=0;
   RHS4(1:NUMNP,1)=0;

%  ---------------------------------
%  Get shape function quadrature data
%  ---------------------------------
   [SF,WT,NUMQPT,NPSIDE] = SFquad(NNPE);

%  -------------------------
%  Create element matrices
%  -------------------------

   for I=1:NUMEL
     QE1(1:NNPE,1)=0.0;
     QE2(1:NNPE,1)=0.0;
     QE4(1:NNPE,1)=0.0;
     S2(1:NNPE,1:NNPE)=0.0;
     rc1=NP(I,:);
%    ---------------------------------------
%    Begin volume quadrature for each element
%    ---------------------------------------
     JEND=NUMQPT(1);

     for J=1:JEND;
```

```
        SFj  = SF(1,:,J); % : nodal point number
        DNDu = SF(2,:,J);
        DNDv = SF(3,:,J);

%         ---------------------------------
%         Determine coordinate and Jacobian
%         ---------------------------------
          XJ=SF(1,:,J)*XORD(rc1)';
          YJ=SF(1,:,J)*YORD(rc1)';
          RJAC(1,1)=DNDu*(XORD(rc1))';
          RJAC(1,2)=DNDv*(XORD(rc1))';
          RJAC(2,1)=DNDu*(YORD(rc1))';
          RJAC(2,2)=DNDv*(YORD(rc1))';
          DETJ=det(RJAC);
          if DETJ <=   0
            fprintf(1,'\n-------------------------')
            fprintf(1,'\n Error in steady.m        ')
            fprintf(1,'\n DETJ =%7e',DETJ          )
            fprintf(1,'\n must be > 0.0'           )
            fprintf(1,'\n-------------------------\n')
            error
          end

%         -----------------------------
%         Determine inverse of Jacobian
%         -----------------------------
          RJACI=inv(RJAC);
%         ------------------------------------------------------
%         Determine derivative of shape functions in X-Y plane
%         ------------------------------------------------------
          DNDX=RJACI(1,1)*DNDu+RJACI(2,1)*DNDv;
          DNDY=RJACI(1,2)*DNDu+RJACI(2,2)*DNDv;
%         ---------------------------------
%         Include user written coefficients
%         RXJ, RYJ, BXJ, BYJ, GVJ, HVJ
%         ---------------------------------
          QE1=QE1+WT(1,J)*c1*SFj'*EPXX(I,J)*DETJ;
          QE2=QE2+WT(1,J)*c1*SFj'*EPYY(I,J)*DETJ;
          QE4=QE4+WT(1,J)*c1*SFj'*EPXY(I,J)*2*DETJ;
          S2=S2+WT(1,J)*c1*SFj'*SFj*DETJ;
          for II=1:NUMEL
             rc2=NP(II,:);
             S11(1:NNPE,1:NNPE)=0.0;
             S12(1:NNPE,1:NNPE)=0.0;
             S14(1:NNPE,1:NNPE)=0.0;
             S22(1:NNPE,1:NNPE)=0.0;
             S24(1:NNPE,1:NNPE)=0.0;
             S44(1:NNPE,1:NNPE)=0.0;
             SS11=0.0;SS12=0;SS14=0;SS22=0;SS24=0;SS44=0;
             for JJ=1:JEND
                 SFjj = SF(1,:,JJ); % : nodal point number
                 DNDu = SF(2,:,JJ);
                 DNDv = SF(3,:,JJ);
                 XJJ=SF(1,:,JJ)*XORD(rc2)';
                 YJJ=SF(1,:,JJ)*YORD(rc2)';
                 RJAC(1,1)=DNDu*(XORD(rc2))';
```

```
                RJAC(1,2)=DNDv*(XORD(rc2))';
                RJAC(2,1)=DNDu*(YORD(rc2))';
                RJAC(2,2)=DNDv*(YORD(rc2))';
                DETJJ=det(RJAC);

                RJACI=inv(RJAC);

                DNDX2=RJACI(1,1)*DNDu+RJACI(2,1)*DNDv;
                DNDY2=RJACI(1,2)*DNDu+RJACI(2,2)*DNDv;

                c11=exp(-((XJ-XJJ).^2+(YJ-YJJ).^2)/Lc^2)*c1*(1-
c1)+c1^2;

                SS11=sum(sum(DNDX'*DNDX2.*G(2*NP(I,:)-1,2*NP(II,:)-
1)));
                SS12=sum(sum(DNDX'*DNDY2.*G(2*NP(I,:)-1,2*NP(II,:))));
                SS14=sum(sum(DNDX'*DNDY2.*G(2*NP(I,:)-1,2*NP(II,:)-
1)+DNDX'*DNDX2.*G(2*NP(I,:)-1,2*NP(II,:))));
                SS22=sum(sum(DNDY'*DNDY2.*G(2*NP(I,:),2*NP(II,:))));
                SS24=sum(sum(DNDY'*DNDY2.*G(2*NP(I,:),2*NP(II,:)-
1)+DNDY'*DNDX2.*G(2*NP(I,:),2*NP(II,:))));
                SS44=sum(sum(DNDY'*DNDY2.*G(2*NP(I,:)-1,2*NP(II,:)-
1)...
                    +DNDX'*DNDY2.*G(2*NP(I,:),2*NP(II,:)-1)...
                    +DNDY'*DNDX2.*G(2*NP(I,:)-1,2*NP(II,:))...
                    +DNDX'*DNDX2.*G(2*NP(I,:),2*NP(II,:))));

                S11=S11+SS11*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
                S12=S12+SS12*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
                S14=S14+SS14*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
                S22=S22+SS22*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
                S24=S24+SS24*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
                S44=S44+SS44*WT(1,J)*WT(1,JJ)*SFj'*SFjj*c11*DETJ*DETJJ;
            end
            K11(rc1,rc2)=K11(rc1,rc2)+S11;
            K12(rc1,rc2)=K12(rc1,rc2)+S12;
            K14(rc1,rc2)=K14(rc1,rc2)+S14;
            K22(rc1,rc2)=K22(rc1,rc2)+S22;
            K24(rc1,rc2)=K24(rc1,rc2)+S24;
            K44(rc1,rc2)=K44(rc1,rc2)+S44;
        end
    end
%     ------------ end of volume quadrature

%     ---------------------------------------------------------------
%     Place completed element matrix in global SK and Q matrices
%     ---------------------------------------------------------------

    RHS1(rc1)=RHS1(rc1)+QE1;
    RHS2(rc1)=RHS2(rc1)+QE2;
    RHS4(rc1)=RHS4(rc1)+QE4;
    K2(rc1,rc1)=K2(rc1,rc1)+S2;

end  % Loop over elements

%  ---------------------------
%  Specify known values of P (traction BC)
```

```
%  --------------------------
   [SF,WT,NUMQPT,NPSIDE] = SFquad(NNPE);
   nx=zeros(NUMNP,1);
   ny=zeros(NUMNP,1);
   ny(1:9)=-1;
   ny(834:841)=-1;
   ny(145:153)=1;
   ny(962:969)=1;
   ny(833)=1;
   ny(577)=-1;
   nx(154:168)=abs(NODES(155:169,2)-
NODES(154:168,2))./((NODES(155:169,2)-
NODES(154:168,2)).^2+(NODES(155:169,1)-NODES(154:168,1)).^2).^.5;
   ny(154:168)=-abs(NODES(155:169,1)-
NODES(154:168,1))./((NODES(155:169,2)-
NODES(154:168,2)).^2+(NODES(155:169,1)-NODES(154:168,1)).^2).^.5;
   ny(169)=-1;
   ny(426:433)=-1;
   nx(562:576)=-abs(NODES(563:577,2)-
NODES(562:576,2))./((NODES(563:577,2)-
NODES(562:576,2)).^2+(NODES(563:577,1)-NODES(562:576,1)).^2).^.5;
   ny(562:576)=-abs(NODES(563:577,1)-
NODES(562:576,1))./((NODES(563:577,2)-
NODES(562:576,2)).^2+(NODES(563:577,1)-NODES(562:576,1)).^2).^.5;
   ny(577)=-1;
   nx(410:424)=abs(NODES(411:425,2)-
NODES(410:424,2))./((NODES(411:425,2)-
NODES(410:424,2)).^2+(NODES(411:425,1)-NODES(410:424,1)).^2).^.5;
   ny(410:424)=abs(NODES(411:425,1)-
NODES(410:424,1))./((NODES(411:425,2)-
NODES(410:424,2)).^2+(NODES(411:425,1)-NODES(410:424,1)).^2).^.5;
   ny(425)=1;
   ny(554:561)=1;
   nx(818:832)=-abs(NODES(819:833,2)-
NODES(818:832,2))./((NODES(819:833,2)-
NODES(818:832,2)).^2+(NODES(819:833,1)-NODES(818:832,1)).^2).^.5;
   ny(818:832)=abs(NODES(819:833,1)-
NODES(818:832,1))./((NODES(819:833,2)-
NODES(818:832,2)).^2+(NODES(819:833,1)-NODES(818:832,1)).^2).^.5;
   ny(833)=1;

   NX=zeros(NUMNP,114);
   NY=zeros(NUMNP,114);
   J=1;
   for I=1:NUMNP
       if (nx(I)^2+ny(I)^2)~=0
           Lamda(I)=J;
           J=J+1;
       end
   end
   npn=zeros(NNPS,1);
   npl=zeros(NNPS,1);
   for I=1:NUMEL
       for J=1:NSPE
%         --------------------------------
%       CHECK IF QUADRATURE IS NECESSARY
%         --------------------------------
```

```
          CHKT=1.0;
          %CHKTY=1.0;
          %clear nps;
          for K=1:NNPS
             J1=NP(I,NPSIDE(J,K));
             CHKT=(nx(J1)^2+ny(J1)^2)*CHKT;
             %CHKTY=CHKTY*ny(J1);
             %nps(K)=NPSIDE(J,K);
             npn(K)=J1;
             npl(K)=Lamda(J1);
          end

          if CHKT ~= 0
%            ---------------------------------------
%            BEGIN SURFACE QUADRATURE ON SIDE J
%            ---------------------------------------
             %nps=[nps,nps+NNPE];
             KEND=NUMQPT(2);
             for K=1:KEND;
                %----------------------------
                % Calculate quadrature point
                % values of parameters and
                % mapping dsdu value.
                %----------------------------
                SF4nK=SF(4,1:NNPS,K);
                SF5nK=SF(5,1:NNPS,K);
                %XK   = SF4nK*XORD(npn)';
                %YK   = SF4nK*YORD(npn)';
                DXDXI= SF5nK*XORD(npn)';
                DYDXI= SF5nK*YORD(npn)';
                NNX=SF4nK'*SF4nK*nx(NP(I,NPSIDE(J,1)));
                NNY=SF4nK'*SF4nK*ny(NP(I,NPSIDE(J,1)));

                %---------------------------------
                % Add quadrature values to integral
                %---------------------------------
                DETJS=sqrt(DXDXI^2+DYDXI^2);
                %Nf=[SF4nK',BLNKs';BLNKs',SF4nK'];
                NX(npn,npl)=NX(npn,npl)+NNX*WT(2,K)*DETJS;
                NY(npn,npl)=NY(npn,npl)+NNY*WT(2,K)*DETJS;

             end % of surface quadrature
          end %  if-statement for quadrature
       end % of loop over element sides
    end

Z=zeros(NUMNP,114);Z0=zeros(114,114);Z1=zeros(114,114);Z2=zeros(114,114
);
    K= [K2/E/R+K11 -K2/E/R*MU+K12 K14 NX Z;-K2'/E/R*MU+K12' K2/E/R+K22
K24 Z NY;K14' K24' K44+K2*2*(1+MU)/E/R NY NX;NX' Z' NY' Z1 Z0;Z' NY'
NX' Z0 Z2];
    F=[RHS1;RHS2;RHS4;zeros(114*2,1)];
    P=K\F;
    cputime-t0
    PP2=P(1+NUMNP:2*NUMNP);
    PP4=P(1+2*NUMNP:3*NUMNP);
    PP1=P(1:NUMNP);
```