LSMearth-EFG coupling: an alternative numerical approach for multi-scale simulations

Osamu Hazama(1), David Place(2), and Hiroshi Okuda(3)

(1)Graduate Student, Dept. of Mechanical Engineering and Materials Science, Yokohama National University, Yokohama, Japan (e-mail: hazama@typhoon.cm.me.ynu.ac.jp , phone: +81-45-339-3875) (2) Senior Research Officer, QUAKES, Dept. of EarthSciences, The University of Queensland, Brisbane, Australia (e-mail: place@earthsciences.uq.edu.au , phone: +61-7 3365 2176) (3) Associate Professor, Dept. of Quantum Engineering and Systems Science, University of Tokyo, Tokyo, Japan (e-mail: okuda@q.t.u-tokyo.ac.jp , phone: +81-3-5841-7426)

Abstract

A new and alternative numerical approach towards efficient and effective studying of the physics involved in the earthquake phenomena was developed. LSMearth, capable of simulating the fracture and failure of the rocks in microscopic scale was coupled with the macroscopic, elasto-static element-free Galerkin model. A coupler was developed to transfer the physical values between the two to describe the deformation. Since the two are written in different programming languages, C++ and F90, all data are transferred to one another through the coupler by initiating a function call by the job controller and/or EFG software, written in F90. This preliminary report illustrates the methodologies implemented for this coupling process and a simple analysis case, which shows to be a promising approach for the future studies.

Introduction

The numerical simulations have become efficient and effective tools for studying the earthquake phenomena. This owes to the very fact in the accelerated advancements made in the computer hardware and in the numerical methods themselves. Yet the earthquake phenomena is still not fully understood due to its complex physical nature.

In order to study the earthquake processes, it is necessary to look at the fault dynamics in microscopic scales as well as in macroscopic scales. Data from observation and laboratory experiments should be properly accounted in the numerical analyses taking into account of many complex physical conditions in both scales of the simulation.

In this work, a preliminary report will be given on multi-scale simulations involving the fault model by coupling together the LSMearth software package developed at QUAKES, University of Queensland, for the microscopic modeling and EFG elastostatics software developed by the first author at Yokohama National University, for the macroscopic modeling. It shall be shown that since neither of the methods employ "mesh"as in the conventional finite elements, multi-scale simulations by coupling of the two methodologies may become an efficient approach for the future studies of earthquake processes through numerical simulations. In this preliminary work, the emphasis is on the numerical coupling of the two methodologies rather than the actual physics involved in the multi-scale simulations, which will be the topic in the very near future.

Overview of Numerical Methodologies

Lattice Solid Model

Lattice Solid Model (LSM) (Mora, 1993[1]) is derived from the molecular dynamics approach where the interactions of the particles, representing grains and rocks, are simulated at the microscopic scales. Like the molecular dynamics, inter-particle potentials are defined, which is used to compute the forces acting on the interacting particles. In addition to these forces, Maxwellian viscosity and friction between the particles are also considered (Mora, 1994[2]).

Newtonian equation of motion is solved for every particle with Velocity-Verlet scheme employed for the integration of the equation of motion with respect to time. This sets the particle positions and velocities into the next discrete time step.

Lattice solid model has found success in numerically simulating realistic fracture and friction behavior of rocks in a microscopic scale. This approach seems to be promising in realistically simulating the earthquake processes.

Element-Free Galerkin Method

Element-Free Galerkin Method (EFGM) (Belytschko, 1994[4]) is a class of so-called "mesh-free" or "meshless" numerical methods which have gained attention and popularity in the last 5 years. As its name suggests, EFG employs the approach of discretizing the Galerkin weak forms of the partial differential equations governing a continuum like its couterpart, the finite elements. However, in the finite elements, element "mesh" is required to discretize the weak forms because shape functions implemented for the spatial interpolation of the funtions are defined element-space-wise. On the other hand, EFG requires no such "mesh", because shape functions are not predefined to a space such as in the finite elements, but rather computed for every sampling point by the Moving Least-Squares (MLS) approximation technique. However, in order to evaluate the spatial integrals of the Galerkin weak forms through such methods as Gaussian quadrature, a spatial partitioning of the continuum domain is necessary.

In this work, the macroscopic model employed is elastostatic, and therefore, a boundary-value problem involving the static equilibrium equation, geometric and traction boundary conditions with elastic constitutive equation (Hooke's Law) is the target to be solved. A principal of virtual work equation, a Galerkin equivalent, shall be discretized by the Moving Least-Squares with a grid called the background cells covering the entire domain to evaluate the spatial integrals by the Gauss-Legendre quadrature (Hazama, 2000[5]).

Multi-scale Simulations by Coupling

Because LSMearth software is written in C++ and EFG software in F90, there is a need to develop a coupler which bridges the two softwares datawise. The following sections briefly describe how the programs exchange data through the coupler and how the simulation is to be run. The coupling strategies described here are similar to that of the coupling carried out by Iizuka *et al* (Iizuka, 2000[3]).

Coupling

In order to couple the micro and macroscopic models, forces and displacements are exchanged between EFG and LSM. Displacements of the LSM particles at the physical interface is interpolated and transferred to EFG nodes via coupler. EFG treats the received displacements as geometric boundary conditions in the proceeding time step. On the other hand, EFG transfers nodal forces at the physical boundaries to the LSM particles via coupler, and LSM uses the forces as boundary conditions in its computations at a given time step. Through this data exchange, the coupling simulation in a micro-macro model deformation is made possible.

Since the EFG receives the displacements at the nodes on the interfaces rather than on the boundary segments, nodal integration over those nodes were carried out to evaluate the displacements as essential boundary conditions.

Job Controller

Job controller is the program main of the LSMearth and EFG softwares written in F90. The main responsibility of the job controller is to call out routines in the coupler, EFG, and LSM, and to control the time step loop. The basic concept is illustrated in Table 1. First, the job controller must call out routines which initializes the models for both EFG and LSM as well as initializing the coupler. As this is completed, the actual physical interfaces between the LSM particles and EFG nodes are defined by the coupler.

```
program main
   call init_efg()
   call init_lsm()
   call init_lsm_efg()
   call init_coupler()

   do
     call analyze_efg()

     do
       call lsm()
     end do
   end do
end program main
```

Table 1: Brief Concept of the Job Controller

Coupler

The coupler has the responsiblity of linking the two software systems. It has access to the data in both EFG and LSM. The simple "get "and "put"functions are defined which allows the access to the coupler from both softwares. The data transferred by these funtions are defined in the coupler, and therefore, can not be changed by the EFG and LSM softwares. Functions "save"and "load"are built into the user program which allows the EFG and LSM softwares to copy the local variable data to or from the coupler-owned variable data.

Definition of Physical Interface

The physical interfaces to be defined by the coupler is carried out by using polygon lists. The EFG software is linked with a CAD (Computer Aided Design) software which allows for it to define the numerical domain. Here, the idea of "layers"will be incorporated in constructing the polygon lists for the definition of the physical interfaces. As illustrated in Fig. 1, the outer polygon, or “layer1 ”is always treated as the outer boundary for the EFG computations. Any subsequent “layers”are considered as “holes”and no computation is considered by the EFG for that space in domain. In these “holes”, the LSM particles will be filled to run dynamic analyses in the microscopic scale. The numbers and numbers enclosed in a circle represent node IDs and polygon segment IDs, respectively.

In order for the coupler to define the interface boundary, EFG writes out the above polygon list out to a file after defining its model in the initialization processes. This file is read by the coupler and the coupler interprets the “holes”as LSM domain. The sample data in Fig. 1 will be interpreted to a polygon list as given in Table 2.

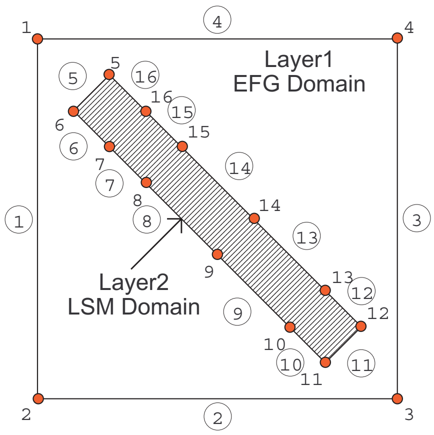


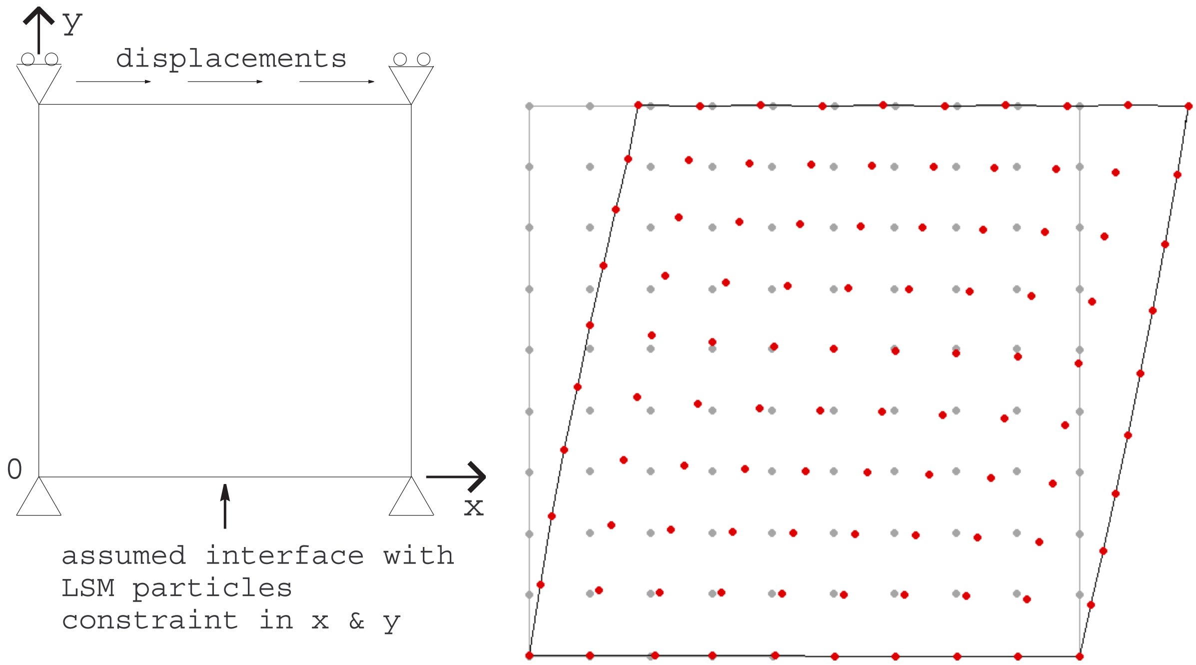
Figure 1: Polygons for Domain and Physical Interface Definitions

16	number of nodes on polygon boundaries
1 0.0000000E+00 1.0000000E+01	node ID, node coordinates x y
2 0.0000000E+00 0.0000000E+00	
3 1.0000000E+01 0.0000000E+00	
⋮	
16 2	number of segments, number of polygons
1 1 0	polygon ID, first node number, EFG domain flag (0)
2 5 1	polygon ID, first node number, LSM domain flag (1)
1 2	ID of nodes making up segment 1
2 3	ID of nodes making up segment 2
⋮	

Table 2: Sample Polygon List Data for Defining Physical Interface (Fig. 1)

Computations

Since EFG receives the displacements from the LSM particles at the nodes rather than at the interface boundary segments, nodal integration scheme for the prescription of the geometric boundary conditions was verified. As in Fig. 2a, a square plate is subjected to shear deformation with the bottom boundaries assumed to be the physical interface with the LSM particles. It was assumed that the LSM particles were holding the nodes in place (0



(a) Domain Model

(b) Illustration of Deformation

Figure 2: Test for Nodal Integration Scheme with LSM Interface Assumption

constraint in both x and y directions). Fig. 2b illustrates the deformation. Gray and red dots depict nodes before and after deformation, respectively. It may be witnessed that the constraint at the bottom boundary agrees well with the assumptions made.

Similar rectangular model was coupled with LSM to verify the deformation in a coupled state. Again, it is subjected to a shear deformation. This time, the bottom boundary is actually coupled with the LSM particles.

A preliminary report of a coupled simulation involving deformations around the fault is also to be presented. Fault zone is modeled using the LSM particles and the surrounding zones are modeled as elastic solids by the EFG.

Concluding Remarks

The coupler interface will allow a multi-scale simulations linking two diffrent numerical approaches: LSMearth in microscopic and EFG in macroscopic scales. As described, the coupler handles the transfer of data between the two softwares written in different programming languages. Through the use of this interface, totally “meshfree”numerical simulation approach was constructed to study the deformation state around the fault model. Since only elasto-static formulation was employed in this study, macroscopic modeling involving viscoelasticity, elasto-plasticity, as well as heat transfer, and dynamic analysis involving wave propagations, are future topics which merits more investigation on the part of the element-free Galerkin.

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