A MULTISCALE METHOD COUPLING NETWORK AND CONTINUUM MODELS IN POROUS MEDIA I – STEADY-STATE SINGLE PHASE FLOW

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Abstract. We propose a numerical multiscale method for coupling a conservation law for mass at the continuum scale with a discrete network model that describes the microscale flow in a porous medium. In this work we focus on coupling pressure equations. Evaluating pressure from a detailed network model over a large physical domain is typically computationally very expensive. We assume that over the same physical domain there exists an effective mass conservation equation at the continuum scale which could have been solved efficiently if the equation was explicitly given. Our coupling method uses local simulations on sampled microscale domains to evaluate the continuum equation and thus solve for the pressure in the full domain. We allow nonlinearity in the network model as well as the mass conservation equation. Convergence of the coupling method is analyzed. In the case where classical homogenization applies, we prove convergence of the proposed multiscale solutions to the homogenized equations. Numerical simulations are presented.

Key words. multiscale, network model, numerical homogenization, porous media flow, heterogeneous multiscale method

AMS subject classifications. 65N99, 65Z05, 76M50

1. Introduction. In this paper, we develop a new multiscale model and algorithm for computing pressure of flow in porous media. The algorithm has the form of the heterogeneous multiscale method (HMM) [25], and couples network models with continuum scale PDE models defined on the same physical domain.

Modeling multi-phase fluid flow in the subsurface is a notoriously difficult challenge. One must account for processes occurring on a broad range of scales; typically different modeling approaches are needed at different length scales so that the underlying physics can be properly described. At the pore scale (with grain size ranging from $\mu m$ to $mm$), direct simulation of Stokes flow in a medium with rich geometry is extremely costly. Model reduction at the pore scale is normally done by mapping the pore space onto a representative network of idealized pores and throats and then modeling fluid displacements as discrete events on the pore-throat network. For overview of network models see [46, 13, 50]. At larger scales (ranging from meters and up), Darcy’s law based on permeability is the most common model. A challenge lies in adequately compressing the pore scale features into the permeability function used in Darcy’s law. The specific micro structure of the pore space frequently plays a critical role in determining macroscopic flow properties, and often cannot be ignored. Continuum models capable of accounting for two scales - the so-called dual porosity models [3, 4, 42] - have been constructed, and some efforts have also been made to...
build hybrid pore scale and continuum models [9, 55]. In [9], Balhoff et al. focused on a scenario in which a pore network domain is connected to a continuum Darcy model for solving single phase fluid flow. In their setting, the network domain and continuum domain are physically disjoint except for a shared interface where information from either domains are exchanged. In [10], the mortar method [5] is used to simplify assumptions and improve the computational complexity.

Coupling of network model and continuous equations has been used by Rossa, D'Angelo and Quarteroni, [49], to model traffic flows in a complex network. In their work, the PDEs at the continuum scale are explicitly derived from network models defined over regular lattice. The coefficients in the PDE can be computed from locally averaging the microscopic solutions. In contrast, in our work, we only assume mass conservation at the continuum level, but otherwise no explicit assumptions on the exact form of the equations. We do not assume regular connectivity in the network models either.

To make our introduction more concrete, consider the following simple setting with a single incompressible fluid at steady state. The fluid velocity \( \mathbf{v} \) depends on pressure \( P \), pressure gradient \( \nabla P \) and the background geological data. The dependence of geological data is described by the location variable \( \mathbf{x} \). Mass conservation implies

\[
\nabla \cdot \mathbf{v}(\mathbf{x}, P, \nabla P) = S(\mathbf{x}),
\]

where \( S \) is a source or sink term. In classical models, the flux velocity is assumed to satisfy Darcy’s law. That is, \( \mathbf{v} \) is proportional to the negative pressure gradient \( -\nabla P \) and \( \mathbf{v} = -\kappa(\mathbf{x})\nabla P \). The positive definite tensor function \( \kappa(\mathbf{x}) \) is called permeability. In this case, equation (1.1) is an elliptic partial differential equation (PDE), and many multiscale methods discuss how to upscale the permeability tensor from finer to coarser scales. The proposed method computes evaluations of \( \mathbf{v} \) and \( P \) directly from simulations using the given detailed pore-scale network models, without assuming or requiring that \( \mathbf{v} \) is linear in \( \nabla P \).

There is a large literature on numerical upscaling from one continuum Darcy equation to another effective Darcy equation whose permeability function has no dependence on the small scales. One type of approaches consists of applying finite element methods with special basis functions that are computed by solving local homogeneous PDEs subject to special boundary conditions. The primitive form of this method can be traced back to the early work of Babuška, Caloz and Osborn [8, 7] who introduced special basis functions for one dimensional elliptic problems with rough coefficients. Hou and Wu [40] generalized this idea to develop the multiscale finite element method (MsFEM) for multi-dimensional problems with multiscale coefficients. The further convergence analysis of the method can be found in [40, 41]. Later on Efendiev, Hou et al. have applied multiscale finite element/volume methods to two-phase flow in porous media problems [29, 30, 23, 21, 1]. For more discussions on the theory and applications of MsFEM, we refer to a recent book by Efendiev and Hou [31].

The upscaled pressure field can be obtained by solving a mass conservation law on coarse grids in a domain decomposition fashion. The transmissibility each coarse cell boundary is typically calculated through a local simulation with generic boundary conditions (i.e. flows in the \( x \) and \( y \) directions). In [20, 19], Chen, Durlofsky et al. proposed a local-global technique to improve the accuracy of this type of upscaling procedure. Global (upscaled) pressure is used to design a better Dirichlet boundary conditions for local simulations, which are used in term to update cell boundary
transmissibility. Global pressure is then updated with new transmissibility. The local simulations and global coarse scale calculation are iterated until a self-consistent solution is achieved. Through coupling global pressure into local simulations, the method improves accuracy significantly even for complicated flow scenarios. The “adaptive local-global” (ALG) upscaling technique[19] increases efficiency by introducing thresholding into the original formulation to avoid repeated calculation of transmissibility for unnecessary blocks and maintain similar accuracy. Our method uses a similar algorithmic structure in coupling macro scale and local scale simulations.

The heterogeneous multiscale method (HMM) [25], introduced by E and Engquist, is a general framework for designing multiscale methods by exploiting special structure of problems. HMM starts with an overall macroscopic model that may miss some constitutive relations for macro variables on the macro grid. The missing quantities and data in the macroscopic model are obtained by solving an accurate microscale model locally with minimal cost. The HMM framework has been applied to several different multiscale applications: material science [44], complex fluids [47], homogenization [28, 2], stochastic ODEs [52, 27], highly oscillatory dynamical systems [24, 34, 6], wave propagation [32]. More details can be found in a review paper by E et al. [26]. Recently, Young and Mitran [54] proposed an HMM-type algorithm to model and compute the deformation of fibrous materials. In the context of homogenization for elliptic problems, in contrast to MsFEM and to increase efficiency, HMM only uses partial information in microscale model to extract missing data and construct approximated homogenized coefficient. Further, in the particular case of homogenization, the algorithm proposed in this paper can be interpreted as a finite volume HMM for homogenization of elliptic problems. In the Appendix, we present a proof of convergence of the solutions computed by the proposed algorithm to the homogenized solutions.

Our methods share conceptual similarities to many of the algorithms mentioned above. For instance, compared to the work of Chen and Durlofsky et al. [20, 19], both methods couple the macro-pressure and micro-pressure through boundary conditions, and iterate until the system match. Both techniques are thus of concurrent type (see [26]) and are not based only on precomputing the effective permeability. Our algorithm differs, however, from most existing methods by coupling different models on different scales and in the sizes of the micro scale domains used in the simulations. Our algorithm couples the given network model to an effective continuum conservation law (continuum model). The elements of a network model are typically in micrometer size range and, depending on the size of the entire model, are representative on millimeter or centimeter scale. (The network model sizes typically considered can be numerically shown to capture a representative elementary volume for permeability of a sandstone or granular medium.) At the length scale ranging from centimeters to a few meters, the effective properties of such networks can be modeled by suitable continuum equations. It is rather reasonable to expect that the flows are effectively one or two dimensional – along the direction of the pressure difference. Hence, while the given pore-scale networks may come from a nonlinear three dimensional system, the effective continuum conservation law can be posed in one, two or three dimensions, depending of the effective properties of the network. Figure 2.2 depicts the coupling of a one dimensional effective model to a three dimensional network and the representative subnetworks. The effective continuum conservation law is not assumed to be linear; i.e. the effective flux can be a nonlinear function of the pressure and the pressure gradient. The proposed algorithm treats all these situation systemati-
cally. In contrast, the typical situations considered by MsFEM or by [20, 19] involve upscaling a given Darcy’s law to another effective Darcy’s law and can ultimately model much larger length scales ($\sim$ km). Of course, in such large length scale, it is unrealistic to expect homogeneity in the underlying medium’s permeability. Thus these algorithms are designed to sample the assumed strong spatial heterogeneity in the media by either building special basis functions with large support size or using large size representative volumes. We point out here that the primary targeted length scale of our proposed algorithm is smaller than that of the other upscaling algorithms. In our considered length scale, it is reasonable to allows for the use of representative subdomain of designated micro scale domain as opposed to exact match of micro and macro scale boundaries.

Finally, we mention a unique feature of our algorithm: it enables the modification of the fine scale model according to the upscaled solutions. Traditionally, the absolute permeability field in reservoir simulations is assumed to be given and unchanged, but in reality it might dynamically change (e.g. due to opening or closing of fractures or infiltration of fine material). Dynamic updates of the permeability field are then needed via local microscopic simulation. The proposed algorithm allows for a new coupling mechanism in which network properties such as conductivities or even the connectivity may be a function of the effective properties that take place at a much larger length scale. This particular feature enables us to incorporate a fracture model in our multiscale model (see Section 3).

2. The HMM scheme for a model problem. In this section, we present and analyze the proposed multiscale coupling algorithm. To simplify exposition, we consider the situation where we impose a significant pressure difference to the network in the $x$ direction and assume that the effective pressure profile at the larger length scale varies only in the $x$ direction. In this simplified setting, it is reasonable to couple the three dimensional network (small scale) model to a one dimensional effective equation involving only $x$ as independent variable. Our method, however, is not limited to only this simplified situation. Coupling network models to multi-dimensional continuum models is presented in Section 2.6.

2.1. Network Models at the Microscopic Scale. Network flow modeling, pioneered by Fatt [35, 36, 37], provides a method to link the microscale description of the medium (topology and geometry) with macroscopic fluid properties. A network model aims at good representation of pore and throat interconnectivity in a porous medium. While pores and throats are depicted via simple geometrical shapes, the models retain a subset of the realistic microscale properties (such as pore/throat size or coordination number distribution) thus, for instance, capturing small scale competition between capillary and viscous forces in multiphase flow. In contrast, in averaging/homogenization approaches, capillary forces are captured only via upscaled relations (capillary-pressure - saturation). Reviews on network flow models by Celia et al. [18] and Blunt et al. [13, 14] have more details on the models and their historical development.

Theoretical predictions of macroscopic two-phase flows in porous media can be achieved by averaging of Navier-Stokes equations on the pore level, assuming appropriate boundary conditions. However, obtaining a closed system of averaged equations requires the introduction of constitutive relations between the different parameters, such as capillary pressure-saturation and relative permeability-saturation. These relations can be obtained (or approximated) from simulations on representative networks. Network models are used, for example, to study relationship among saturation, capillary
Fig. 2.1. An example of the correspondence of a block of grains and a network model. In the network model, the grains are neglected, the pores are represented by balls (nodes) and the throats are represented by cylindrical tubes (segments).

pressure and interfacial area [46], predict properties such as permeability [17, 45], imbibition and drainage curves [39], phase distributions, relative permeability [45, 51, 53] and wettability [22].

In network models, pores are simply represented as nodes and throats as links (in the simplest form, they are cylindrical tubes). The nodes and links are usually depicted by vertices and edges respectively. Thus a network model has a topology of a graph. However, as each pore has a physical location, we shall refer a network that models a medium in a $d$ dimensional domain as a $d$ dimensional network. See Figure 2.1 for an illustration of a two dimensional network. In this paper, we maintain the following assumption on the length of the throats in the network:

Assumption 2.1. The length of the throats in the network are bounded by a small positive parameter which we denote by $\epsilon$.

Consider a three dimensional network over the domain $[x_L, x_R] \times [y_1, y_2] \times [z_1, z_2]$. For convenience, we number the nodes in the domain. We denote by $I^{(0)}$ the index set containing all the indices of the nodes lying in the interior of the network domain. Let $I_i$ contain the indices of nodes which are connected to node $i$; in other words, each index in $I_i$ corresponds to a node which is connected to node $i$ by a throat. Let $p_i$ denote the pressure inside pore $i$ and for each $j \in I_i$, let $c_{ij}$ denote the conductance of the throat which connects node $i$ and the node $j$.

The conductance for a Newtonian fluid in a cylindrical throat is computed exactly using Hagen-Poiseulle solutions and is given by

$$c_{ij} = \frac{\pi r^4}{8l\mu},$$

where $r$ is the radius and $l$ the length of the throat, and $\mu$ is the viscosity of the fluid. For more general fluids, the conductance $c_{ij}$ may be a nonlinear function depending on the nearby pressure $p_i$ and $p_j$.

The flux from node $i$ to node $j$ is then $c_{ij}(p_i - p_j)$, and the law of mass conservation leads to

$$\sum_{j \in I_i} c_{ij}(p_i - p_j) = s_i, \quad i \in I^{(0)},$$

where $s_i$ is the sink or source in the pore $i$. System (2.1) should be coupled with suitable boundary conditions on the boundary nodes, typically emulating Dirichlet,
periodic or Neumann conditions. In most practical cases, the fluid is assumed incompressible and \( s_i = 0 \) except at injection or production pores.

We impose Dirichlet boundary conditions on the left \((x = x_L)\) and the right \((x = x_R)\) faces and periodic boundary condition (or no flow condition) on the remaining parts of the boundary. Let \( I_L \) and \( I_R \) denote respectively the index set for nodes lying on the left and the right side face of the domain. The Dirichlet boundary conditions are imposed by assigning \( p_i = P_R \) for all \( i \in I_R \) and \( p_i = P_L \) for all \( i \in I_L \).

When there is no source term present in the network, the total flux \( f \) through the left face is the same as the flux through the right

\[
f = \sum_{i \in I_L} \sum_{j \in I_i} c_{ij} (p_i - p_j) = - \sum_{i \in I_L} \sum_{j \in I_i} c_{ij} (p_i - p_j). \tag{2.2}
\]

The function \( f \) is the total flow rate in the \( x \)-direction caused by the pressures \( P_L, P_R \) applied to the left face and the right face. Therefore, \( f \) is the sum of the fluxes through the throats crossing any planar section that is parallel to the \( x \)-\( z \) plane. We can define the permeability \( \kappa \) of the network by

\[
\kappa = \frac{k}{A},
\]

where \( A \) is the area of the left face, and the velocity \( \mathbf{v} \) in (1.1) satisfies the Darcy’s law:

\[
\mathbf{v} = \frac{f}{A} = \frac{-k(P_R - P_L)}{A\delta} = -\kappa \frac{P_R - P_L}{x_R - x_L}.
\]

See Lemma A.2 for more detail. When the network model is nonlinear, the maximal-minimal principle still holds, but \( q \) may not be a constant function and \( f(P_L, P_R) \) depends on \( P_L \) and \( P_R \) nonlinearly.

### 2.2. Macroscopic Continuum Model

As in the previous subsection, we consider a network model over the domain \([x_L, x_R] \times [y_1, y_2] \times [z_1, z_2]\), with Dirichlet conditions on the boundaries at \( x_L \) and \( x_R \), and periodic boundary condition (or no flow Neumann) on the other four faces. Let \( B_3(x) \) denote the subdomain \([x - \delta/2, x + \delta/2] \times [y_1, y_2] \times [z_1, z_2]\) and \( \Sigma(x; \delta) \) be the boundary of \( B_3(x) \). By integrating (1.1) over \( B_3(x) \) and using the boundary conditions, we have

\[
\int_{B_3} \mathbf{S} \, dv = \int_{B_3} \mathbf{v} \, dv = \int_{\Sigma} \mathbf{v} \cdot \mathbf{n} \, ds = F_{\Sigma_R} - F_{\Sigma_L}, \tag{2.4}
\]
where $F_{\Sigma_n}$ and $F_{\Sigma_L}$ are the fluxes through boundaries at $x + \delta/2$ and $x - \delta/2$ respectively. Dividing both sides of (2.4) by $\delta$ and taking the limit as $\delta \to 0$ we obtain a one-dimensional macroscopic equation

$$\frac{d}{dx} F = \lim_{\delta \to 0} \frac{1}{\delta} \int_{B_\delta(x)} Sdv \equiv Q(x), \quad x \in (x_L, x_R),$$

(2.5)

from a three-dimensional network model in microscale. The macroscopic domain becomes simply $[x_L, x_R]$ and the unknowns are the macroscopic pressure $P$ and flux $F$. The macroscopic pressure $P$ can be viewed as an average pressure of small scale pressure $p$ on the cross section $\Sigma(x; 0^+)$. We assume the flux $F$ is a function of pressure $P$, pressure gradient $P_x$, and location $x$. Equation (2.5) is posed with given boundary values $P(x_L) = P_L$ and $P(x_R) = P_R$.

We apply a finite volume discretization for (2.5). Let $N$ be the number of partitions of $[x_L, x_R]$ and $\Delta x = (x_R - x_L)/N$, $x_l = x_L + l \Delta x$. Let $\hat{P}_l$ be the approximation of $P(x_l)$ and $\hat{F}_{l+\frac{1}{2}}$ be the approximation of the flux $F(x_{l-\frac{1}{2}})$. The finite volume discretization of (2.5) is to find $P_0, P_1, P_2, ..., P_{N-1}, P_N$ such that $P_0 = P_L, P_N = P_R$ and

$$F_{l+\frac{1}{2}} - F_{l-\frac{1}{2}} = \int_{x_l-\frac{1}{2}}^{x_{l+\frac{1}{2}}} Q dx \equiv Q_l \Delta x \quad \text{for } l = 1, 2, ..., N - 1.$$  

(2.6)

Functional relations of the discrete fluxes $F_{l+\frac{1}{2}}$ and the macroscopic pressures $P_l$ are to be approximated from the coupling of (2.6) and the network model.

**2.3. Coupling of the macroscopic model and the network model.** Figure 2.2 shows a schematic representation of coupling macroscale and microscale models. For each grid node $x_l$, we choose a subdomain $B_\delta(x_{l-\frac{1}{2}})$. We refer the corresponding portion of our network over this subdomain as the local network centered at $x_{l-\frac{1}{2}}$. The boundary conditions for each local network are given as in Section 2.1,
except that the values for the Dirichlet conditions are determined by the macroscopic pressures. The details of the coupling are summarized below:

- The macroscopic flux $F_{l-\frac{1}{2}}$ is defined as the flux, denoted by $\tilde{f}_{l-\frac{1}{2}}$, through the corresponding local network, induced by the Dirichlet boundary conditions at $x = x_{l-\frac{1}{2}} \pm \delta/2$, determined by $P_{l-1}$ and $P_l$. Thus, the macroscopic flux if formally a function of the two pressure values; i.e.

$$F_{l-\frac{1}{2}} = F_{l-\frac{1}{2}}(P_{l-1}, P_l) = \tilde{f}_{l-\frac{1}{2}}. \tag{2.7}$$

- The Dirichlet boundary conditions for the subdomain $B_\delta(x_{l-\frac{1}{2}})$ at $x_{l-\frac{1}{2}} \pm \delta/2$ are defined by the values of the macroscopic pressure at the corresponding locations. At the discretization level, they are approximated by linear interpolation of $P_l$ and $P_{l-1}$ on $[x_{l-1}, x_l]$ to define an approximation of the pressure $P$ at $x_{l-\frac{1}{2}} \pm \delta/2$. Thus, the flux through the local network is a function depending on two macroscopic pressure values and the center of the subdomain

$$\tilde{f}_{l-\frac{1}{2}} = \tilde{f}_{l-\frac{1}{2}}(P_{l-1}, P_l) = f(x_{l-\frac{1}{2}}, P_{l-1}, P_l), \tag{2.8}$$

where $f$ is the function defined by (2.2) in Section 2.1. More precisely, the Dirichlet boundary conditions at $x_{l-\frac{1}{2}} \pm \delta/2$ are $P_{l-\frac{1}{2}, L}$ and $P_{l-\frac{1}{2}, R}$ defined by $P_{l-\frac{1}{2}} = (P_{l-1} + P_l)/2$, and

$$P_{l-\frac{1}{2}, L} = P_{l-\frac{1}{2}} - D^+ P_{l-1}(\delta/2), \quad P_{l-\frac{1}{2}, R} = P_{l-\frac{1}{2}} + D^+ P_{l-1}(\delta/2),$$

where $D^+ P_{l-1} = (P_l - P_{l-1})/\Delta x$ is the standard divided centered differencing on $P_{l-1}$.

- The size of the local network, denoted by $\delta$, is chosen according to the relative strength of heterogeneity in the network conductance. For networks with weak heterogeneity in the $x$ direction in the macroscopic length scale, it is reasonable to use small $\delta$. For networks with strong heterogeneity, $\delta$ is enlarged. Our algorithm places no restriction that $\delta$ has to be small; $\delta$ can be taken to be $x_l - x_{l-1}$ so that the local networks overlap at $x_l$.

- The source term $\int_{x_{l-\frac{1}{2}}}^{x_{l+\frac{1}{2}}} Q \, dx = \int_B Sdv$ is obtained by summing all source term $s_i$ in each pores inside subdomain $B$.

In the coupling method described above, the flux $F$ is evaluated for any given pressures $P_{l-1}$ and $P_l$, via simulations using local networks. The formal equations (2.6), (2.7), and (2.8) for the macroscopic pressure $P_l$ may be nontrivial to solve as the relation between $F_{l-\frac{1}{2}}$, $P_{l-1}$ and $P_l$ are not available explicitly. In particular, the Newton’s method is not applicable and thus an alternate root finding scheme is required. We propose a quasi-Newton-like scheme in next section.

### 2.4. Macro-Micro Iterative Scheme

From the previous section, we see that the flux through a point in the macroscopic domain can be evaluated from the flux through the corresponding local network. We need to find the pressure values in the macroscopic domain from the computed fluxes. The main difficulty is that no convenient analytical relation between the macroscopic flux $F$ and the pressure $P$ is available (or assumed). In the following discussion, we first assume that there is no source term in the system. The case where the source term is nonzero will be discussed in Section 2.4.1.
At the discrete level, we want to solve the following equations for $P_l$:

$$F(x_{l+\frac{1}{2}}, P_{l+\frac{1}{2}}, D^+ P_l) = \hat{f}_{l+\frac{1}{2}}(P_l, P_{l+1}). \quad (2.9)$$

$$D^- F(x_{l+\frac{1}{2}}, P_{l+\frac{1}{2}}, D^+ P_l) = Q_l \Delta x, \quad l = 1, 2, \ldots, N-1, \quad (2.10)$$

with the boundary condition $P_0 = P_L, P_N = P_R$. See Figure 2.2 for a diagram. We propose to solve the above coupled equations by simple iterations roughly as follows: The left hand side of Equation (2.10) will be approximated using $F_l^{(n+1)}$ as well as $P_l^{(n)}$. We start out from a fundamental assumption that

$$F(x, P, P_x) = f(x, P, P_x) = 0, \quad \text{whenever } P_x = 0.$$ 

Suppose further that $F$ is smooth, then mean value theorem suggests that

$$F(x, P, P_x) = F_{P_x}(x, P, \xi)P_x,$$ 

where $F_{P_x}$ refers to the partial derivative of $F$ with respect to third variable and $\xi \in [0, P_x]$ is an intermediate value, which depends on $P$ and $x$. Therefore, we use

$$F_{P_x}(x, P, \xi) \approx \hat{f}_{l+\frac{1}{2}}(P_l, P_{l+1})/D^+ P_l =: -K_{l+\frac{1}{2}}(P_l, P_{l+1}). \quad (2.12)$$

Hence, the iterative scheme becomes:

$$-D^- \left(K_{l+\frac{1}{2}}(P_l^{(n)}, P_{l+1}^{(n)})D^+ P_l^{(n+1)}\right) = Q_l \Delta x. \quad (2.13)$$

We next describe details of the algorithm. We shall see, from (2.17) and (2.20), that our proposed scheme can be interpreted as a type of quasi-Newton method at the network simulations. In the following, we summarize our proposed algorithm. We refer the readers to the Appendix B for a convergence proof of this algorithm.

**Algorithm 2.2.** \textit{Start with an initial guess $P^{(0)} = [P_0^{(0)}, P_1^{(0)}, \ldots, P_N^{(0)}]^T$ with $P_0^{(0)} = P_L, P_N^{(0)} = P_R$ and $P_l^{(0)} \neq P_{l-1}^{(0)}$ for all $l = 1, 2, \ldots, N$. A conventional choice is to generate the initial guess from linear interpolation of the boundary conditions. That is, $P_l^{(0)} = (\Delta x(x_{l+1/2} - x_L)/x_{l+1/2} - x_L) + P_L$.}

\textit{For $n = 0, 1, \ldots}$

1. Solve the local network problems over $B_3(x_{l-\frac{1}{2}}), l = 1, 2, \ldots, N$ with boundary conditions described in Section 2.3.

2. Evaluate $F_{P_x}^{(n)} = \hat{f}_{l-\frac{1}{2}}(P_{l-1}^{(n)}, P_{l}^{(n)})$ for $l = 1, 2, \ldots, N$.

3. Compute the effective parameter $K_{l-\frac{1}{2}}(n) := K_{l-\frac{1}{2}}(P_{l-1}^{(n)}, P_{l}^{(n)})$ and construct the matrices $K_{l-\frac{1}{2}}^{(n)}$ and $h^{(n)}$ as defined below:

If $P_{l}^{(n)} \neq P_{l-1}^{(n)}$:

$$K_{l-\frac{1}{2}}^{(n)} = F_{l-\frac{1}{2}}^{(n)} \frac{\delta}{(P_{l-\frac{1}{2}, L}^{(n)} - P_{l-\frac{1}{2}, R}^{(n)})} = -\frac{F_{l-\frac{1}{2}}^{(n)}}{D^+ P_{l-1}^{(n)}}, \quad (2.14)$$

otherwise, we estimate $K_{l-\frac{1}{2}}^{(n)}$ by

$$K_{l-\frac{1}{2}}^{(n)} = -\hat{f}_{l-\frac{1}{2}}(P_{l-1}^{(n)}, P_{l-1}^{(n)} + \epsilon P) \frac{\Delta x}{\epsilon P},$$
where \( \epsilon_P \) is a small positive number (we choose \( 10^{-12} \) in our numerical experiments).

\[
K^{(n)} = \begin{pmatrix}
K_{\frac{1}{2}}^{(n)} + K_{\frac{3}{2}}^{(n)} & -K_{\frac{1}{2}}^{(n)} & 0 & \cdots & 0 \\
-K_{\frac{1}{2}}^{(n)} & K_{\frac{1}{2}}^{(n)} + K_{\frac{3}{2}}^{(n)} & -K_{\frac{1}{2}}^{(n)} & \ddots & \vdots \\
0 & -K_{\frac{1}{2}}^{(n)} & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & -K_{\frac{1}{2}}^{(n)} & K_{\frac{1}{2}}^{(n)} + K_{\frac{3}{2}}^{(n)} \\
\end{pmatrix},
\]

\[
h^{(n)} = [Q_1 + K_{1-\frac{1}{2}}^{(n)} P_L / \Delta x^2, Q_2, \ldots, Q_{N-2}, Q_{N-1} + K_{N-\frac{1}{2}}^{(n)} P_R / \Delta x^2]^T. \tag{2.15}
\]

4. Update \( P^{(n+1)} \) by solving the linear equation

\[
K^{(n)} P^{(n+1)} = \Delta x^2 h^{(n)}; \tag{2.16}
\]

i.e.

\[
P^{(n+1)} = (1 / \Delta x^2) K^{(n)} P^{(n)} - h^{(n)} = (1 / \Delta x^2) G(P^{(n)}), \tag{2.17}
\]

where

\[
G(P^{(n)}) = \frac{1}{\Delta x^2} K^{(n)} P^{(n)} - h^{(n)} = [D^+ P^{(n)}_{1-\frac{1}{2}} - Q_1, D^+ P^{(n)}_{2-\frac{1}{2}} - Q_2, \ldots, D^+ P^{(n)}_{N-1-\frac{1}{2}} - Q_{N-1}]^T. \tag{2.18}
\]

Stop when a chosen numerical convergence criterion is met.

The proposed iterative scheme has several good properties. The matrices \( K^{(n)} \) are symmetric positive definite and tridiagonal. Therefore the linear equation (2.16) can be solved in \( O(N) \) operations (for example by Cholesky decomposition), and the solution \( P^{(n+1)} \) satisfies max-min property. That is, \( P^{(n+1)}_l \) is between the boundary value \( P_L \) and \( P_R \). This guarantees the proposed macro-micro iterative scheme will never blow up numerically.

Let us comment briefly on situation when \( P^{(n)}_l = P^{(n)}_{l-1} \). When there is no source term inside the network model, it is not hard to see \( P^{(n)}_l - P^{(n)}_{l-1} \neq 0 \) for all \( l \) and \( n \) unless boundary the conditions \( P_L \) and \( P_R \) are the same. However, when there is a nonzero source (or when considering 2D and 3D macroscopic models discussed in Section 2.4.1), \( P^{(n)}_l - P^{(n)}_{l-1} \) can be zero for some \( l \) and \( n \).

For general flux functions \( F_{l-\frac{1}{2}}, \) (2.17) still holds in our method, but \( 1 / \Delta x^2 K \) is not equal to the Jacobian of \( G \). Recall that

\[
F_{l-\frac{1}{2}}(P_l, P_{l-1}) = \hat{F}_{l-\frac{1}{2}}(P_{l-1}, P_l) = -K_{l-\frac{1}{2}}(P_l, P_{l-1}) D^+ P_{l-1}
\]

for some nonnegative function \( K_{l-\frac{1}{2}}(P_l, P_{l-1}) \). If \( K_{l-\frac{1}{2}} \) is differentiable with respect to \( P_l \) and \( P_{l-1} \), a direct computation shows that the Jacobian of \( G \) is

\[
J = \frac{\partial G}{\partial P} = \frac{1}{\Delta x^2} K + \frac{1}{\Delta x^2} A, \tag{2.20}
\]
where $A$ is tridiagonal with

$$A_{l,k} = \left( P_l - P_{l+1} \right) \frac{\partial K_{l+\frac{1}{2}}}{\partial P_k} - \left( P_{l-1} - P_l \right) \frac{\partial K_{l-\frac{1}{2}}}{\partial P_k}, \quad \text{for } k = l-1, l, l+1 \quad (2.21)$$

Therefore our method is a quasi-Newton’s method derived by discarding the matrix $A$ in Jacobian of $G$.

Let us summarize a few key points of the proposed algorithms presented above.

- The effective continuum equation is discretized as in (2.6), leading to a nonlinear system of equations for the macroscopic pressure $P_l$.
- Local network simulations are used to evaluate the nonlinear fluxes $F$ at points designated by the discretization (2.6).
- Since no explicit analytic form is available for the macroscopic flux $F$, in order to solve (2.6) for $P_l$, the proposed scheme utilizes an idea from Taylor expansion of the flux function.
- In this setup, the solution of the discretized macroscopic equation is the root of $G$. In Appendix D, we present a numerical experiment which demonstrates the efficiency of the proposed method in solving the nonlinear equation $G(P)=0$.

### 2.4.1. Presence of Source Terms

In previous discussions, we assume that the source term is zero network model. This is not the case when there are injection and production the network model, and in this case, the flux through the local network may not vanish even when $P_l = P_{l-1}$. Consequently, we can not apply our macro-micro iteration directly.

For convenience of the following discussion, we denote by $\hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l, s_{l-\frac{1}{2}})$ the flux resulted from the presence of nonzero source terms, and by $\hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l)$ the flux through the same domain but with the source term set to zero. Of course, ultimately, the macroscopic flux is defined by $F_{l-\frac{1}{2}}(P_{l-1}, P_l) = \hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l, s_{l-\frac{1}{2}})$.

When the network model is linear, we can modify the equation to apply our algorithm. By linearity of the solution of the network model, we have

$$\hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l, s_{l-\frac{1}{2}}) = \hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l) + \hat{f}_{l-\frac{1}{2}}(0, 0, s_{l-\frac{1}{2}}), \quad (2.22)$$

where $f(P_{l-1}, P_l)$ is the flux obtained from network model with zero source as defined in Section 2.1.

The decomposition (2.22) is not valid in the case of nonlinear networks with source terms. Suppose that for a given macro pressure, $P_{l-1}$ and $P_l$, we solve the corresponding local nonlinear network model over $B_\delta(x_{l-\frac{1}{2}})$ and obtain the pressure $\tilde{p}_i$ at node $i$. With the computed pressure $\{\tilde{p}_i\}$, we define an equivalent linear network model by assigning a posteriori the linear the conductance $\tilde{c}_{ij}$ the value of the nonlinear conductance $c(\tilde{p}_i, \tilde{p}_j)$. Denote by $\hat{f}_{l-\frac{1}{2}}^L(P_{l-1}, P_l, s_{l-\frac{1}{2}}; \{\tilde{c}_{ij}\})$ the flux through this new linear network model with conductance $\tilde{c}_{ij}$, the Dirichlet boundary conditions $P_{l-1}$, $P_l$, and the source term $s_{l-\frac{1}{2}}$. Obviously, with $\tilde{c}_{ij}$ defined by the solution of the local nonlinear network, we have the following identity

$$\hat{f}_{l-\frac{1}{2}}(P_{l-1}, P_l, s_{l-\frac{1}{2}}) = \hat{f}_{l-\frac{1}{2}}^L(P_{l-1}, P_l, s_{l-\frac{1}{2}}; \{\tilde{c}_{ij}\})$$
$$= \hat{f}_{l-\frac{1}{2}}^L(P_{l-1}, P_l; \{\tilde{c}_{ij}\}) + \hat{f}_{l-\frac{1}{2}}^L(0, 0, s_{l-\frac{1}{2}}; \{\tilde{c}_{ij}\}),$$

where $\hat{f}_{l-\frac{1}{2}}^L(P_{l-1}, P_l; \{\tilde{c}_{ij}\})$ is tridiagonal with

$$A_{l,k} = \left( P_l - P_{l+1} \right) \frac{\partial K_{l+\frac{1}{2}}}{\partial \tilde{p}_k} - \left( P_{l-1} - P_l \right) \frac{\partial K_{l-\frac{1}{2}}}{\partial \tilde{p}_k}, \quad \text{for } k = l-1, l, l+1.$$
where \( f_{l-rac{1}{2}}^L(P_{l-1}, P_l; \{\bar{c}_{i,j}\}) = f_{l-rac{1}{2}}^L(P_{l-1}, P_l, 0; \{\bar{c}_{i,j}\}) \). Under this setting \( f^L \) satisfies the property \( f_{l-rac{1}{2}}^L(P_{l-1}, P_l; \{\bar{c}_{i,j}\}) = 0 \) when \( P_{l-1} = P_l \), and thus the approximation (2.12) can be applied to recover pressure from the values of the fluxes.

We summarize the macro-micro iterative scheme for nonlinear network model with nonzero source as the following.

**Algorithm 2.3.** Start with an initial guess \( P^{(0)} = [P_0^{(0)}, P_1^{(0)}, \ldots, P_N^{(0)}]^T \) with \( P_0^{(0)} = P_L, P_N^{(0)} = P_R \) and \( P_l^{(0)} \neq P_{l-1}^{(0)} \) for all \( l = 1, 2, \ldots, N \).

For \( n = 0, 1, \ldots \)

1. Solve nonlinear network model to get obtain the pressure \( \{p_i^{(n)}\} \) and evaluate the flux \( \hat{f}_{l-rac{1}{2}} (P_{l-1}^{(n)}, P_l^{(n)}, s_{l-rac{1}{2}}) \).
2. Define a linear network model by the conductance \( c_{i,j}(p_{i}^{(n)}, p_{j}^{(n)}) \) to compute \( \hat{f}_{l-rac{1}{2}}^L(0, 0, s_{l-rac{1}{2}}; \{\hat{c}_{i,j}^{(n)}\}) \) and define
\[
\hat{f}_{l-rac{1}{2}}^{(n)} = \hat{f}_{l-rac{1}{2}} (P_{l-1}^{(n)}, P_l^{(n)}, s_{l-rac{1}{2}}) - \hat{f}_{l-rac{1}{2}}^L(0, 0, s_{l-rac{1}{2}}; \{\hat{c}_{i,j}^{(n)}\})
\]
3. Compute the effective parameter
\[
K_{l-rac{1}{2}}^{(n)} = -\frac{\hat{f}_{l-rac{1}{2}}^{(n)}}{D^+ P^{(n)}}
\]
and construct the matrix \( K^{(n)} \) as in (3) and \( h^{(n)} \) defined by
\[
h_l^{(n)} = \begin{cases} 
Q_l - D^+ f_{l-rac{1}{2}}^{(n)} + K_{l-rac{1}{2}}^{(n)} P_l \Delta x^{-2}, & l = 1 \\
Q_l - D^+ f_{l-rac{1}{2}}^{(n)}, & 1 < l < N \\
Q_N - D^+ f_{N-rac{1}{2}}^{(n)} + K_{N-rac{1}{2}}^{(n)} P_R \Delta x^{-2}, & l = N,
\end{cases}
\]
where \( f_{l-rac{1}{2}}^{(n)} = f_{l-rac{1}{2}}^L(0, 0, s_{l-rac{1}{2}}; \{\hat{c}_{i,j}^{(n)}\}) \) obtained in (2).
4. Update \( P^{(n+1)} \) by solving the linear equation
\[
K^{(n)} P^{(n+1)} = \Delta x^2 h^{(n)},
\]
Stop when a chosen numerical convergence criterion is met.

The proof of convergence of the iterative scheme is similar to Algorithm 2.2.

### 2.5. An Alternative on the Boundary Conditions for Local Network Model

In general, errors coming from the Dirichlet boundary conditions for local network simulations increase as the number blocks increases, while the errors coming from the discretization of the macroscale model. In some simulations, the former dominates the total errors, and this explains the why lower number of blocks resulted in smaller errors. This is mainly a one dimensional phenomenon and thus not so important in realistic simulations. In classical homogenization theory, the homogenized coefficient is obtained by solving cell problems and the boundary condition for the cell problem is periodic after subtracting a linear function [11]. Using the similar idea, we can incorporate the macroscopic pressure \( P_l \) and \( P_{l-1} \) with the flux function \( F_{l-rac{1}{2}} \).

Given macroscopic pressures \( P_l \) at \( x_l \), and \( P_{l-1} \) at \( x_{l-1} \), we create a microscopic pressure profile \( p^L \) on the sampling subdomain \( B_\delta(x_{l-rac{1}{2}}) \) by linearly interpolating \( P_l \) and \( P_{l-1} \) in \( x \)-direction. To determine the macroscopic flux \( F_{l-rac{1}{2}} \), we solve the
pressure $\tilde{p}$ such that $\tilde{p}$ satisfies the equation (2.1) on $B_\delta$ and $\tilde{p} - p^L$ satisfies periodic condition on the boundary of $B_\delta$. The flux $\tilde{f}_{l-\frac{1}{2}}$ is then defined by

$$\tilde{f}_{l-\frac{1}{2}} = \sum_{i \in L_{-}} \sum_{j \in L_{i}} c_{ij}(\tilde{p}_i - \tilde{p}_j),$$

and $F_{l-\frac{1}{2}} = \tilde{f}_{l-\frac{1}{2}}$. Notice that under this construction, $\tilde{p}$ needs not to be the same value on the left or right faces of $B_\delta$ and the artificial boundary effect should be reduced. We shall refer this boundary condition as the "linearly adjusted periodic boundary condition."

By a small modification of Lemma A.2, the solution $\tilde{p}$ is always solvable and unique up to a constant if the network system is linear. We determine the unique solution by choosing $\tilde{p}$ such that the average of $\tilde{p}$ is $P_{l-\frac{1}{2}, L} = P_{l-\frac{1}{2}} - D^+ P_{l-1}(\delta/2)$ on the left face of $B_\delta$ and the average of $\tilde{p}$ on the right face is $P_{l-\frac{1}{2}, R} = P_{l-\frac{1}{2}} + D^+ P_{l-1}(\delta/2)$, automatically by this choice. We also have that $\tilde{f}(P_{l-1}, P_l) = -kD^+ P_{l-1}$ for some constant function $k$. Hence the macro-micro iteration scheme converges in one iteration.

2.6. Multi-Dimensional Models. In this section, we describe how our method is applied to couple multi-dimensional continuum equations with multi-dimensional networks.

We start with the conservation law (1.1) posed in a rectangular domain with suitable boundary conditions. We use a finite volume discretization to the PDE. Divide the domain into $N_1 \times N_2$ coarse blocks. Let $x_{i,j}$ be the center of a block, and $V$ be the corresponding control volume. See Figure 2.3 for a diagram. Let $F_N, F_S, F_W$, and $F_E$ denote the fluxes through the four edges of $V$. Then (1.1) implies that

$$\oint_{\partial V} \mathbf{v} \cdot \mathbf{n} ds = F_N + F_S + F_W + F_E = \bar{S}(x_{i,j}) \text{Vol}(V), \quad (2.23)$$

where $\bar{S}$ is the mean of the source term inside $V$.

We first consider the case in which $S \equiv 0$. Again, the flux $F$ across each edge is evaluated as $\tilde{f}$ coming from local network simulations on a $\delta \times \delta$ size sampling domain.
with some appropriate boundary conditions from given pressure $P$. For instances, $F_E$ and $F_N$ are defined formally by

$$F_E = v_{i+\frac{1}{2},j} \cdot n_x \Delta y = \hat{f}^{(x)}(P_{i,j}, P_{i+1,j}, P_{i,j+1}, P_{i+1,j+1}, P_{i,j-1}, P_{i+1,j-1})(\Delta y/\delta),$$

$$F_N = v_{i,j+\frac{1}{2}} \cdot n_y \Delta x = \hat{f}^{(y)}(P_{i,j}, P_{i,j+1}, P_{i+1,j}, P_{i+1,j+1}, P_{i-1,j}, P_{i-1,j+1})(\Delta x/\delta),$$

where $\hat{f}^{(x)}$ and $\hat{f}^{(y)}$ are flux evaluations from the local network simulations described below. The boundary conditions used in the local network simulations are determined by the pressure on nearby grid nodes that are shown as the arguments of $\hat{f}^{(x)}$ and $\hat{f}^{(y)}$. In the following discussion, we only present the detail on $F_E$ at $x_{i+\frac{1}{2},j}$. There is no difficulty in computing the other fluxes in similar fashion.

As in the one dimensional case, an explicit algebraic formula for the macroscopic flux $F$ as a function of pressure and pressure gradient is not readily available. However, formulas (2.11) and (2.13) can be generalized easily since $v = (v_1, v_2) = 0$ when $\nabla P = 0$. Taylor expansion shows

$$v_1(x, P, \nabla P) = \partial_{P_x} v_1(x, P, \xi_1, \xi_2) P_x + \partial_{P_y} v_1(x, P, \xi_1, \xi_2) P_y,$$  

(2.24)

where $(\xi_1, \xi_2)$ are the intermediate values. Then the flux $\hat{f}^{(x)}$ can be approximated by

$$\hat{f}^{(x)}(P_{i,j}, P_{i+1,j}, P_{i,j+1}, P_{i+1,j+1}, P_{i,j-1}, P_{i+1,j-1}) \approx ((\partial_{P_x} v_1) P_x + (\partial_{P_y} v_1) P_y) \delta,$$

and the pressure gradient $\nabla P$ is approximated by forward and central difference of $P$; i.e. $P_x \approx D^+_{x} P_{i,j}$ and $P_y \approx D^0_{y} P_{i+\frac{1}{2},j}$, where $P_{i+\frac{1}{2},j} = (P_{i,j} + P_{i+1,j})/2$ and

$$D^0_{y} P_{i+\frac{1}{2},j} = \frac{P_{i+\frac{1}{2},j+1} - P_{i+\frac{1}{2},j-1}}{2\Delta y} = \frac{(P_{i+1,j+1} + P_{i,j+1}) - (P_{i+1,j-1} - P_{i,j-1})}{4\Delta y}.$$  

The flux $\hat{f}^{(x)}$ is evaluated from the local network simulation over $B_0(x_{i+\frac{1}{2},j})$ with the linearly adjusted periodic boundary conditions which can be found in [33] or [32]. More precisely, we impose the condition that $p - p^E$ is periodic on the sampling domain $B_0$; here

$$p^E(x) = U_{i+\frac{1}{2},j} \cdot (x - x_{i+\frac{1}{2},j}) + P_{i+\frac{1}{2},j}$$  

(2.25)

with the vector $U_{i+\frac{1}{2},j} = [D^+_{x} P_{i,j}, 0]T$, is a linear interpolant of the nearby Macroscopic pressure values. The flux $\hat{f}^{(x)}$ is then computed according to (2.2) by the microscopic pressure $p$. Another choice of boundary condition for $p$ is the Dirichlet boundary condition: $p = p^L$ on the boundary of $B_0$.

The "coefficients" $\partial_{P_x} v_1$ and $\partial_{P_y} v_1$ are approximated by the additional local network simulations with $U_{i+\frac{1}{2},j}$ in (2.25) by $[D^+_{x} P_{i,j}, 0]^T$ and $[0, D^0_{y} P_{i+\frac{1}{2},j}]^T$ respectively. More precisely, we define $K^{1,1}_{i+\frac{1}{2},j}$ and $K^{1,2}_{i+\frac{1}{2},j}$ as following

$$\partial_{P_x} v_1 \approx K^{1,1}_{i+\frac{1}{2},j} = \hat{f}^{(x)}(P_{i,j}, P_{i+1,j}, 0, 0, 0, 0)/(\delta D^+_{x} P_{i,j}),$$

$$\partial_{P_y} v_1 \approx K^{1,2}_{i+\frac{1}{2},j} = \hat{f}^{(x)}(P_{i+\frac{1}{2},j}, P_{i+\frac{1}{2},j+1}, P_{i,j+1}, P_{i+1,j+1}, P_{i,j-1}, P_{i+1,j-1})/(\delta D^0_{y} P_{i+\frac{1}{2},j}).$$  

(2.26)
The other coefficients \( K_{i,j}^{1,1}, K_{i,j}^{1,2}, K_{i,j}^{2,1}, K_{i,j}^{2,2} \) are defined analogously.

Now we are ready to describe our Macro-micro iterations. For a given macroscopic pressure \( P_{i,j}^{(n)} \), we compute the coefficients

\[
(K_{i+\frac{1}{2},j}^{1,1})^{(n)}, (K_{i+\frac{1}{2},j}^{1,2})^{(n)}, (K_{i,j+\frac{1}{2}}^{2,1})^{(n)}, (K_{i,j+\frac{1}{2}}^{2,2})^{(n)}
\]

as in (2.26). The updated macroscopic pressure \( P_{i,j}^{(n+1)} \) is obtained by solving the sparse linear system

\[
F_{N}^{(n)} + F_{S}^{(n)} + F_{W}^{(n)} + F_{E}^{(n)} = 0,
\]

where

\[
F_{E}^{(n)} = \left((K_{i+\frac{1}{2},j}^{1,1})^{(n)} D_{i+\frac{1}{2},j}^{y} P_{i,j}^{(n+1)} + (K_{i+\frac{1}{2},j}^{1,2})^{(n)} D_{i+\frac{1}{2},j}^{x} P_{i,j}^{(n+1)}\right) \Delta y,
\]

\[
F_{N}^{(n)} = \left((K_{i,j+\frac{1}{2}}^{2,1})^{(n)} D_{i,j+\frac{1}{2}}^{y} P_{i,j}^{(n+1)} + (K_{i,j+\frac{1}{2}}^{2,2})^{(n)} D_{i,j+\frac{1}{2}}^{x} P_{i,j}^{(n+1)}\right) \Delta x.
\]

Similar to case involving one dimensional macroscopic model, the coefficients \( K \) are constant when the network model is linear, and therefore the iteration converges in one step. For nonlinear networks, the Macro-Micro iteration is a quasi-Newton type method. Let \( \mu(i,j) \in \mathbb{N} \) be an enumeration of the grid nodes \((i,j)\), and \( G \) be the function whose \( \mu \)th component is \( G_{\mu}(\mathbf{P}) = F_{\mu,N} + F_{\mu,S} + F_{\mu,W} + F_{\mu,E} \), where the fluxes are computed around the control volume centered at the \( \mu \)th grid node. Then the proposed model is to find \( \mathbf{P} \) such that \( G(\mathbf{P}) = 0 \), and the iterative scheme can be written analogously to (2.17). The matrix \( \mathbf{K} \) is an approximation of the Jacobian of \( G \) and the convergence result can be showed by a modification on \( A \) of proof of Algorithm 2.2.

When there is non-zero source present in the network model, the local flux \( f^{(x)} \) and \( f^{(y)} \) involve the network source term \( \mathbf{s} \). However, the nonlinearity induced by the source term \( \mathbf{s} \) can be removed as in Section 2.4.1.

3. Fracturing of soft sediments. We propose a simple model to simulate propagation of a fracture in a soft (unconsolidated) sediment. The purpose is to give an example of a network scale process that is not easily represented by an effective equation at the continuum scale, and to show the potential of coupling fluid and solid mechanics.

Pumping highly pressurized fluid into a sediment can cause some throats (fluid pathways) to widen, and thereby allows the fracturing fluid to enter and extend the fracture further into the formation. In our model, fractures are represented as those throats with very high conductance, while the network connectivity remains fixed. This simplified view is intuitively correct in unconsolidated sands.

If a throat, such as the one depicted in the center of Figure 3.1, is filled with fluid, the pore pressure acts both in normal direction to the grain walls (normal stress, shown in solid arrows), as well as parallel to them (shear stress, shown in dash arrows).

The throat depicted will open wider if the total of normal forces pushing the grain labelled \( Gr_{1} \) upwards, and the grain \( Gr_{2} \) downwards, is larger than total of the shear forces acting on both of the grains [43, 48]. Since all forces act on the surface of the same area (length in 2D) \( a \), when the balance is made over all of the normal (solid arrows) forces that act in \( y \) direction and divided by \( a \), we obtain the stress

\[
\sigma_{N} = -\frac{1}{2} (\sigma_{N}^{(1)} + \sigma_{N}^{(2)}),
\]
Fig. 3.1. Illustration for computing stress using local information. Pore space (gray) and grains (white) near the throat connecting pore \((i, j)\) and pore \((i+1, j)\). Pore centers are marked with circles. Normal forces to grain surfaces exerted by pore pressure are depicted with solid arrows, shear forces exerted on grains by viscous forces in motion are shown by the dashed arrows.

where

\[
\sigma_N^{(1)} \approx (p_{i,j+1} - 2p_{i,j} + p_{i,j-1}), \quad \sigma_N^{(2)} \approx (p_{i+1,j+1} - 2p_{i+1,j} + p_{i+1,j-1}).
\]

The shear stresses (dash arrows) acting in \(y\) direction on the two grains above and below the throat are equal to \(2\sigma_N\) in this case. The throat widens if the total stress is larger in magnitude than some critical value \(G_C\), that is \(G = a(\sigma_N + \sigma_T) > G_C\), where \(a\) is the length of the throat. The latter is similar to the concept of the crack extension force from plane elasticity [43, 48], and we will use the same name for it.

Note that in general, the normal and shear forces would also be balanced by gravity acting on each grain as well as the effect of earth stresses (confinement). A simple way of incorporating earth stresses in the network setting can be found in [48]. In our simple network, however, the grains do not touch and thus there is no way to transmit those stresses throughout the grain network. We thus impose limitations that mimic confinement effects as follows.

In our model on local network level, we modify the radii of the throats according to their extension force value. A throat is characterized as a part of fracture when its radius is close to a predefined value \(r_{\text{max}}\); this large size of radius leads to large conductance. If a pore is connected to a throat that is identified as part of a fracture, then the pore is called a fracture node. Further, in each iteration, we check the crack extension force \(G\) of each throat that is connected to a fracture node. In case that \(G > G_C\) for such a throat, we update its radius \(r\) by \(r = H(G)\). Otherwise, its radius stays the same as before. Here we choose

\[
H(G) = r_{\text{max}} \frac{2}{\pi} \tan^{-1}\left(\frac{G - G_C}{s}\right) \quad \text{for} \quad G > G_C,
\]

where \(r_{\text{max}}\) is the maximum conductance value used in the simulation and \(s\) is a suitable scaling. The conductance of this throat is then updated according to its new radius. Notice that we only update the conductance of throats connected to a fracture node and the resulting fracture is always a connected path.

We assume that once fracture is formed, it will not close afterwards. Therefore, in our algorithm, the radius is only updated when the proposed value \(r_{\text{new}}\) is bigger
than previous one $r_{\text{old}}$. That is

$$r_{\text{new}} = \max\{r_{\text{old}}, H(G)\}.$$  

Finally, subsurface formations are under confining pressure (dependent on the depth) and cannot expand freely. In order to simulate this behavior, we confine the radii of throats by restricting the sum of the radii in each column and each row to be less than a given constant. That is, if we denote the radius of the throat connecting pore $\text{(i, j)}$ and pore $\text{(i+1, j)}$ by $r_{i+\frac{1}{2}, j}$, pore $\text{(i, j)}$ and pore $\text{(i, j+1)}$ by $r_{i,j+\frac{1}{2}}$, then $\sum_j r_{i+\frac{1}{2}, j}$ and $\sum_i r_{i,j+\frac{1}{2}}$ are bounded above for all $i$ and $j$. Therefore only certain number of throats in each row and column can be part of a fracture. If the sum of the proposed radii exceed the restriction in certain column, we reassign radii to satisfy the constraint. We update throats according to the order of radii in previous step in each column and row since larger conductance is easier to expand. See Figure 3.2 for simulations with different parameters.

4. Numerical Experiments. In the following experiments, we compare the flux $F_D$ and the pressure $P_D$ computed from direct full simulation on whole network model with the flux $F_H$ and the pressure $P_H$ computed by the proposed multiscale algorithm. In Experiments 1, 2 and 6 which involve one dimensional macroscopic models, the flux $F_D$ at $x_j$ is evaluated by summing the flux through the throats that cross the section $x = x_j$. The pressure $P_D$ at a macro grid node $x_j$ is calculated by averaging the values of fine scale pressure over the network cross section $x = x_j$. In Experiments 3, 4 and 5 which involve two dimensional macroscopic models, the pressure $P_D$ is obtained by taking fine scale pressure at coarse grid nodes, and the flux $F_D$ is calculated by summing the flux through the throats crossing each edge of the control volume $V$. That is, we compare $F_N$, $F_W$, $F_S$, $F_E$ obtained from multiscale
simulation with the flux computed from direct full simulation. The relative errors of flux $e_F$ and of pressure $e_P$ are defined by

$$e_F = \frac{\|F_H - F_D\|}{\|F_D\|}$$

and

$$e_P = \frac{\|P_H - P_D\|}{\|P_D\|}.$$  

where $\|\cdot\|_\infty$ is the supreme norm of vectors.

**Experiment 1. (Linear flux)** We present results on coupling a one dimensional macroscopic model to a two dimensional network with linear flux. We created a network model that has $1001 \times 21$ nodes arranged in $[0,1000] \times [0,20]$. In the network, each node is connected by 6 nearby nodes and the length of throats are 1 unit in horizontal and vertical direction, and are $\sqrt{2}$ unit in diagonal direction. The radii of the throats are randomly generated from the uniform distribution $[(1-\lambda)r_0, (1+\lambda)r_0]$ and the conductance is set to $c_{ij} = \frac{\pi r^4}{8 \mu}$. We choose $r_0 = 0.01$, $\lambda = 0.5$, and $\mu = 1$. In the simulations using the proposed multiscale algorithms, we divide the domain into $N$ blocks, each of the dimension $\delta \times 20$, so that the center of each block corresponds to the node $x_\delta$ described in Section 2.3. At the microscopic level, we experimented with a few local networks with different sizes.

We fix $\delta = 10,15,20$ and set $N = 5,10,20,30$ to test the convergence of the proposed algorithm. We first impose the Dirichlet boundary condition in the $x$-direction: $p = 100$ on the left hand side and $p = 0$ on the right hand side, and periodic boundary condition in $y$ direction. We run 1000 realizations of the radius of each throat to obtain the corresponding conductance $c_{ij}$. The averaged relative errors $e_P$ and $e_F$ obtained from different $N$ and $\delta$ are listed in Table 4.1. We observe that both errors, computed by using Dirichlet boundary conditions, are well controlled for each parameter. The pressure error decreases as the number of blocks $N$ increases or the sampling size $\delta$ increases, but the flux error is mainly controlled by sampling size $\delta$.

The flux error is significantly improved if the *linearly adjusted boundary condition* is used instead. In Figure 4.1, we present the relative errors, computed by using the linearly adjusted boundary condition, as a function of $N\delta$ in log-log plot. The numerical results suggest the error $e_P \sim (N\delta)^{-\alpha}$ and $e_F \sim (N\delta)^{-\beta}$ with $\alpha$ close to 0.59 and $\beta$ close to 0.58. This implies that for fixed $\delta$ (or $N$) both errors are convergent as $N$ (or $\delta$) increases.

The flux errors in relation to the refinement of macroscopic grids as shown in Table 4.1 is mainly a one dimensional phenomenon. In general, it is easier to implement Dirichlet boundary condition, especially for unstructured and complicated network models. In simulations involving higher dimensional macroscopic domains, Dirichlet and linearly adjusted periodic conditions yield comparable convergent errors than periodic boundary condition in simulation.

**Experiment 2. (Three dimensional network from sphere packing)** In this experiment, we use a sphere packing algorithm to generate a 3D network model. The macroscopic model is still one dimensional. Sphere packings are common models used for describing sandstones, and the permeability estimates from the resulting networks compare well to Fontainebleau sandstone (Bryant et al. [16]). The sphere packing of 1020 spheres shown on the left hand side of Figure 4.2 comes from experimental measurements of grain locations in a disordered packing (Finney [38]). This network contains 4,109 pores and 7,551 throats as depicted in the subfigure on the right side of Figure 4.2.

The physical domain of the network is $[-8,8]^3$ and each sphere has a normalized radius of 1. The boundary conditions are $P = 10$ on the left hand boundary, $P = 0$
**Table 4.1**

The relative pressure error \(e_P\) and relative flux error \(e_F\) of Experiment 1 by using 1D-model with \(N\) blocks and \(\delta \times 20\) sampling domains.

<table>
<thead>
<tr>
<th>(N)</th>
<th>(\delta = 10)</th>
<th>(\delta = 15)</th>
<th>(\delta = 20)</th>
<th>(\delta = 10)</th>
<th>(\delta = 15)</th>
<th>(\delta = 20)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.0348</td>
<td>0.0284</td>
<td>0.0240</td>
<td>0.0936</td>
<td>0.0626</td>
<td>0.0487</td>
</tr>
<tr>
<td>10</td>
<td>0.0267</td>
<td>0.0217</td>
<td>0.0185</td>
<td>0.0883</td>
<td>0.0585</td>
<td>0.0440</td>
</tr>
<tr>
<td>20</td>
<td>0.0195</td>
<td>0.0151</td>
<td>0.0122</td>
<td>0.0864</td>
<td>0.0556</td>
<td>0.0403</td>
</tr>
<tr>
<td>30</td>
<td>0.0157</td>
<td>0.0115</td>
<td>0.0086</td>
<td>0.0864</td>
<td>0.0554</td>
<td>0.0412</td>
</tr>
</tbody>
</table>

**Fig. 4.1.** Log-log plot of the relative error of pressure \(e_P\) (left) and flux \(e_F\) (right) versus different total lengths of the sampling domain \(N\delta\) by using the linearly adjusted periodic boundary condition. Four different color lines stand for different number of blocks \(N\).

on the right hand side boundary and no flow for the rest of faces. The distribution of the throats is shown in Figure 4.3, and the mean throat radius is 0.2943 with standard deviation 0.1091. In this simulation, we consider linear flux model and use 1D continuous model. We divide the domain into \(N\) blocks, each of dimension \(\delta \times 16 \times 16\), and fix \(\delta = 0.8, 1.2, 1.6\) and \(N = 5, 8, 10\). Note that the network in this experiment is unstructured and we use linear interpolation of coarse pressure to determine the boundary condition of the sampling domains. Since the network model is defined on a graph with an unstructured grid, the pressure \(P_D\) can not be calculated by the usual way. The pressure \(P_D\) at a macro grid node \(x_j\) is obtained by averaging the fine scale pressure values in the region \([x_j - 0.5, x_j + 0.5] \times [-8, 8]^2\). The errors are given in Table 4.2.

The error of pressure is within a reasonable size for all choices of \(N\) and \(\delta\). The flux error \(e_f\) seems larger than the error in Experiment 2 since the network is unstructured and more heterogeneous than our previous examples. However, when \(N = 5\) and \(\delta = 0.8\), for instance, only total 1007 pores and 2795 throats are used in the multiscale model computation. If we sample the entire network (\(N = 10\) and \(\delta = 1.6\)) the error of both pressure and flux is well-controlled. This shows our scheme can be applied to a complicated network model.

**Experiment 3.** (Two dimensional problem with three disconnected channels with large conductance) Consider a two dimensional network model with \(1001 \times 1001\) pores located on a regular lattice with physical domain \([-0.5, 0.5] \times [-0.5, 0.5]\). Each grid node in the lattice is connected to six nearby pores as we de-
Table 4.2
The relative pressure error $e_P$ and relative flux error $e_F$ of Experiment 2 by using 1D-model with $N$ blocks and $\delta \times 16 \times 16$ sampling domains.

<table>
<thead>
<tr>
<th>$\delta = 0.8$</th>
<th>$\delta = 1.2$</th>
<th>$\delta = 1.6$</th>
<th>$\delta = 0.8$</th>
<th>$\delta = 1.2$</th>
<th>$\delta = 1.6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N = 5$</td>
<td>0.0694</td>
<td>0.0531</td>
<td>0.0542</td>
<td>2.1973</td>
<td>1.2766</td>
</tr>
<tr>
<td>$N = 8$</td>
<td>0.0546</td>
<td>0.0412</td>
<td>0.0387</td>
<td>1.0572</td>
<td>0.4627</td>
</tr>
<tr>
<td>$N = 10$</td>
<td>0.0429</td>
<td>0.0316</td>
<td>0.0257</td>
<td>0.4469</td>
<td>0.1254</td>
</tr>
</tbody>
</table>

Fig. 4.2. (Left) Sphere packing used for construction of the 3D network model in Experiment 2 (Right) Resulting network of pores (shown as spheres) and throats (shown as cylinders).

Picted in Experiment 2. The radius of each throat is a random number chosen from uniform distribution on $[(1 - \lambda)r_0, (1 + \lambda)r_0]$ with $r_0 = 0.01$, $\lambda = 0.5$, except three channels and the length of each throat is 0.001; see Figure 4.4. The channels are composed by horizontal segment connecting pores $(i, j)$ to $(i + 1, j)$, $i \in [1, 400]$ and $j \in [245, 255]$ for the first channel, $i \in [301, 700]$ and $j \in [495, 505]$ for the second channel and $i \in [601, 1000]$ and $j \in [745, 755]$ for the second channel. The radius in the channels is $10r_0$. The pressure corresponding to this network model does not approximate to parallel lines. If we use 1D-model with 5 blocks full sampling to simulate this network model, the relative error of flux is around 2000%. This large error is caused by misinterpreting connection of 3 channels. In 1D-model, each sampling region has a high conductance channel penetrated through, and therefore the regenerative parameter is very high. The induced coarse scale in 1D system has all larger parameters connected together. Three disconnected channels becomes connected and penetrate through the whole region in 1D model, and therefore the computed macroscopic flux is over estimated. To resolve the issue, we need a multi-dimensional macroscopic model.

We divide the domain into $N \times N$ blocks and use $\delta \times \delta$ local network to estimate the macroscopic flux $F$ on each edge of the control volume and apply the proposed 2D model and algorithm. In Table 4.3, we list the relative pressure error $e_P$ and relative flux error $e_F$ for different numbers of coarse blocks and different sampling domain size. We can see the flux and pressure in 2D-model is significantly improved from the results obtained from 1D model. Notice that the errors decrease as $N$ increase even the our error analysis in Appendix C is not applied in this case. The pressure and flux errors are less than 10% for $N = 20$ and $\delta = 0.005$. We only use such few information to capture the macro scale behavior correctly. The errors are large when $N = 5$, and 10 because in these cases the sampling domains do not cover the top and bottom
channels. The resulted representative parameter $K$ only capture one channel. When we increase number of coarse blocks to 20, three channels have been captured. The coarsening parameter exhibits 3 disconnected channel and the coarse scale pressure contour present the similar behavior to the network scale pressure. This numerical example shows full macroscopic model can capture the coarse scale information more accurate than 1D model.

**Experiment 4. (Homogenization to an anisotropic elliptic equation)**
In this experiment, we testify the proposed macroscopic flux and iterative algorithm satisfy the results under the classical homogenization setting. Consider a network model comes from the discretization of the elliptic PDE:

$$-\nabla \cdot (a_\epsilon(x) \nabla u(x)) = 0, \quad x \in [0,1] \times [0,1]$$

with oscillatory coefficient $a_\epsilon(x) = a(x/\epsilon)$, where

$$a(x) = \sin(4x_1) + 0.1 \sin 2\pi(x_1 + 1.41x_2) + 0.1 \cos 2\pi x_2 + 1.20001.$$

Notice that this choice of $a$ leads to an anisotropic homogenized equation. The anisotropic is defined by the effective diffusion tensor $\hat{A}$ whose eigenvectors do not align with vectors formed by connecting grid nodes. With this feature, we are able to test if our proposed multiscale algorithm captures the anisotropy.
Table 4.3

The relative pressure error $e_p$ and relative flux error $e_f$ of Experiment 3 by using 2D-model with $N \times N$ blocks and $\delta \times \delta$ sampling domains.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\delta = 0.005$</th>
<th>$\delta = 0.01$</th>
<th>$\delta = 0.02$</th>
<th>$\delta = 0.005$</th>
<th>$\delta = 0.01$</th>
<th>$\delta = 0.02$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.2580</td>
<td>0.2522</td>
<td>0.2475</td>
<td>0.4558</td>
<td>0.4744</td>
<td>0.4758</td>
</tr>
<tr>
<td>10</td>
<td>0.2912</td>
<td>0.2744</td>
<td>0.2764</td>
<td>0.3444</td>
<td>0.3575</td>
<td>0.3670</td>
</tr>
<tr>
<td>20</td>
<td>0.0665</td>
<td>0.0697</td>
<td>0.0634</td>
<td>0.1022</td>
<td>0.0714</td>
<td>0.0629</td>
</tr>
<tr>
<td>40</td>
<td>0.0558</td>
<td>0.0542</td>
<td>0.0546</td>
<td>0.0620</td>
<td>0.0410</td>
<td>0.0305</td>
</tr>
</tbody>
</table>

Fig. 4.5. The relative error in pressure versus the number of coarse blocks. The left figure is the case when $\epsilon = 0.001$ and the right figure is when $\epsilon = 0.0001$. The dash line represents $y = 1/N^2$.

We discretize the domain into $600 \times 600$ squares and each vertex represents a pore and each edge represents a throat. The conductance of the throat is the value of $a$ at the middle point of the throat. We apply the Dirichlet boundary condition $u(x) = (x_1 + 1)^2(x_2 + 1)^2$ on the boundary of the microscale network domain. The solution of the network model is a numerical approximation of the solution of (4.1). We discretize the network model into $N \times N$ coarse blocks and use $\delta \times \delta$ sampling domain $B_\delta$ to obtain macroscopic pressure $P$ by our macro-micro algorithm. We use periodic boundary condition obtained from macro pressure in local network simulation.

We choose $\epsilon$ to be $0.001$ and $0.0001$, the sampling length $\delta$ to be $0.01$, $0.0167$, and $N$ to be $6, 8, 10, 12, 15, 20, 30, 40$ and compare the value of micro-pressure $p$ with macro-pressure $P$ at the same position. The relative error in pressure $e_p$ is defined as before. See Figure 4.5 for results.

We can observe that $e_p$ is convergent to 0 as $N$ increases before the error is about size $\epsilon$, and convergence is of second order. From our error analysis in Appendix C, we know the error is control by both macroscale and microscale discretization error and homogenization error. Macroscale discretization error is of order $1/N^2$ and homogenization error is of $\epsilon$. When $N$ is large enough, the error is dominated by homogenization and can not be controlled by increasing $N$. This coincides with the error analysis we have in Appendix C.

Because of the choice of the constant 1.41 inside the sinus function, the sampling domains does not coincide with the cell problems exactly and the estimated coefficients are different for each sampling domain. However, the error is still smaller by using $\delta = 0.01$ than using $\delta = 0.167$. This is because when $\delta = 0.01$, the sampling size is an integer multiple of $\epsilon$ for both $\epsilon = 0.001$ and $\epsilon = 0.0001$.

**Experiment 5. (Two dimensional nonlinear radial flow)** Consider a two
Table 4.4

<table>
<thead>
<tr>
<th>N</th>
<th>$\delta = 0.012$</th>
<th>$\delta = 0.016$</th>
<th>$\delta = 0.02$</th>
<th>$\delta = 0.012$</th>
<th>$\delta = 0.016$</th>
<th>$\delta = 0.02$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.0650</td>
<td>0.0630</td>
<td>0.0619</td>
<td>0.3272</td>
<td>0.2634</td>
<td>0.1849</td>
</tr>
<tr>
<td>10</td>
<td>0.0642</td>
<td>0.0606</td>
<td>0.0414</td>
<td>0.1594</td>
<td>0.1343</td>
<td>0.1046</td>
</tr>
<tr>
<td>20</td>
<td>0.0593</td>
<td>0.0524</td>
<td>0.0407</td>
<td>0.0873</td>
<td>0.0748</td>
<td>0.0724</td>
</tr>
</tbody>
</table>

Table 4.4

The relative pressure error $e_P$ and relative flux error $e_F$ of Experiment 5 by using 2D-model with $N \times N$ blocks and $\delta \times \delta$ sampling domains.

Dimensional network model with $501 \times 501$ pores located on a regular lattice over the physical domain $[-0.5, 0.5]^2$. Each grid node in the lattice is connected to four nearby pores. The radius of each throat is a random number chosen from the uniform distribution on $[(1 - \lambda) r_0, (1 + \lambda) r_0]$ with $r_0 = 0.01$, $\lambda = 0.5$, and the length of each throat is set to 0.002.

The flux $f_{ij}$ in the network model is given by [12]:

$$f_{ij} = \frac{\pi r^4}{16 \mu l} \left( \frac{p_i^2 - p_j^2}{p_j} \right).$$

The source term in each pore is given by $10^{-8} \times \phi(\frac{r}{r_0})$, where

$$\phi(x) = \begin{cases} \exp(-\frac{1}{1-x^2}), & x < 1 \\ 0, & x \geq 1 \end{cases},$$

and $r$ is the distance between the pore and the origin. We set $p = 2$ on the boundaries of the full network. The resulting pressure has radial contours.

We divide the domain into $N \times N$ blocks and use $\delta \times \delta$ local networks to estimate the macroscopic flux $F$ on each edge of the control volume and apply the proposed 2D model and algorithm. We list the relative pressure error $e_P$ and flux error $e_F$ for different numbers of coarse blocks and different sampling domain sizes in Table 4.4.

Each full network model simulation uses around 30 fixed point iterations, and takes around 3 hours to get convergent pressure on a moderate laptop running at 2.3 GHz. In the simulations using the proposed algorithm with 20 coarse blocks and sampling size $\delta = 0.02$, at most 5 iterations is needed for compute each $K$ from solving local network problems, and around 10 iterations is needed for outer loop to obtained convergent values of $P^{(n)}_{ij}$. Within 8 minutes, the multi scale algorithm converges. Our simulation is capable of producing results with less than 10% relative errors while sampling only 16% of the full network ($N^2 \delta^2 = 0.16$).

**Experiment 6. (Multiscale simulations with the fracture model in local networks)** In this experiment, we incorporate our quasi-static fracture development model for two dimensional networks into the multiscale algorithm. We consider a full linear network consisting of $1001 \times 21$ pores and edges taken from a regular Cartesian lattice over the domain $[0, 1000] \times [0, 20]$. We set the source term $s_i \equiv 0$ in the network and impose Dirichlet condition with $p = 100$ and $p = 0$ on left and right hand side of the full network, and periodic boundary condition in the $y$-direction. The radii of throats are initially randomly generated from the uniform distribution on $[(1 - \lambda) r_0, (1 + \lambda) r_0]$ with $r_0 = 0.01$ and $\lambda = 0.5$, we choose the viscosity $\mu = 1$.

In the presented multiscale simulation, we divide the whole network into 10 blocks, and evaluate the macroscopic fluxes by simulations using local networks obtained from
the 101 × 20 pores centering at each block. To track the development of fracture growth correctly, the sampling domain is entire block, i.e., δ = 100. We apply the quasi-static fracture development model described in Section sec:fracture initially only to the first (the left most) local network. The conductance connecting pore (1, 11) to pore (2, 11) in the first local network is set to be \( r_{\text{max}} = 10r_0 = 0.1 \) as the initialization of a fracture. Then we develop fracture in the first block until it stops or reaches the right hand side of the block. In each iteration, we update coarse pressure \( P \) by solving upscaled equation with the network model that is dynamically updated by the fracture development.

When fracture reaches the right hand side of the first block, we continue the fracture to the second block. We initialize a fracture in the second block by setting the radii of the throats connected to the fracture nodes in the second local network to be 10\( r_0 \) and perform the same fracture development simulation in first two blocks. Inductively, we continue this process until the fracture development stops or reaches the right side of the full network domain. We run 1000 realizations of initial conductances and compare the macro pressure and the flux obtained from fracture development simulation with direct full simulation. The average pressure error \( e_p \) is 0.0554 and flux error \( e_f \) is 0.0907. Figure 4.6 shows an example of snapshots of fracture obtained from full and multiscale simulation of one particular realization.

5. Conclusion. In this paper, we present a multiscale algorithm which computes the effective continuum length scale fluxes of given pore-scale network models. Conventional upscaling algorithms typically assume a single physical model posed on the same physical domain for the different scales. The proposed algorithm shares certain similarities to these upscaling algorithms in similar settings. Nevertheless, our algorithm has several unique features as follows:

- The algorithm couples the given network (pore scale) model to an effective continuum conservation law (continuum model). The effective continuum conservation law is not assumed to be linear; i.e. the effective flux can be a nonlinear function of the pressure and the pressure gradient.
- While the given pore-scale networks may come from a nonlinear three dimensional system, the effective continuum conservation law can be posed in one, two or three dimensions, depending on the application. The proposed algorithm treats all these situations systematically. As we have seen in Experiment 2, the effective performance of a three dimensional network model is computed via coupling thin slices of the networks (local networks) to a continuum conservation law.
- The proposed algorithm allows for a new coupling mechanism in which net-
work properties such as conductivities or even the connectivity may be a function of the effective properties that take place at a much larger length scale. This particular feature enables us to incorporate a dynamic fracture model in our multiscale model.

- In numerical examples and by homogenization analysis we showed that the proposed multiscale coupling method indeed computes with some detailed features of the network model with a computational efficiency which is closer to that of simulations with only continuum equations.

Appendix A. Properties of Network models. We present two simple properties of network models in this section.

**Lemma A.1.** Suppose that any two nodes in the domain are connected by a continuous path of throats, and the conductance $c_{ij} > 0$ for each $i$ and $j \in I_i$. Then the pressure $p$ satisfies the maximal and minimal principle, i.e.,

$$\max_{i \in I} \{p_i\} = \max_{i \in J / I(0)} \{p_i\}, \quad \text{and} \quad \min_{i \in I} \{p_i\} = \min_{i \in J / I(0)} \{p_i\}.$$ 

**Proof.** By contradiction, suppose that maximum is attained at an interior node; i.e. $\max_{i \in I(0)} \{p_i\} > \max_{i \in J / I(0)} \{p_i\}$. Let $I_M$ denote the largest index set containing all index $i$ such that $p_i = \max_{i \in I(0)} \{p_i\}$. Then $I_M \subseteq I(0) \subset I$ and there exist indices $i_s \in I_M$ and $j_s \in I_*$ such that $j_s \notin I_M$. Since $p_{i_s} = \max_{i \in I(0)} \{p_i\}$ and $c_{ij} > 0$, we have

$$\sum_{j \in I_*} c_{i_s, j} (p_{i_s} - p_j) \geq c_{i_s, j_s} (p_{i_s} - p_{j_s}) > 0$$

which contradicts to (2.1). The proof of the minimal principle is analogous. $\square$

**Lemma A.2.** Suppose any two nodes in the network can be connected by a continuous path of throats, and the conductance $c_{ij} > 0$ for all $i, j \in I_i$. Then there exists a unique solution $\{p_i\}_{i \in I(0)}$ satisfying (2.1) and the Dirichlet boundary conditions at the left and the right network boundaries, and periodic condition in the remaining faces.

1. Then there exists a unique solution $\{p_i\}_{i \in I(0)}$ satisfying (2.1) and the Dirichlet boundary conditions at the left and the right network boundaries, and periodic condition in the remaining faces.

2. If the conductance $c_{ij}$ is also independent of $p_R$ and $p_L$, then there exists a nonnegative constant $k$ depending only on $c_{ij}$ such that the flux take the form

$$f = -k(p_R - p_L)/\delta,$$

where $\delta$ is the distance between left face and right face.

**Proof.** Rewritten (2.1) as

$$Cp = b, \quad (A.1)$$

where $p$ is the vector whose entries are $p_i$ for $i \in I(0)$ and $b$ is determined by the boundary conditions $P_R$ and $P_L$. Since $C$ is a square matrix independent of $p$, it suffices to show that $C$ is injective. Suppose $b = 0$, then it is easy to see $P_L = P_R = 0$. Max-Min principle (Lemma A.1) implies $p = 0$. Hence $C$ is invertible and $p$ is uniquely solvable.

Let $p_*$ be the solution of (A.1) with $P_R = 1$ and $P_L = 0$ and $p$ be the solution of (A.1) with arbitrary $P_R$ and $P_L$. By linearity of the system (A.1), $p = (P_R - P_L)p_* + P_L$. Denoting the flux resulting from the boundary values $P_R, P_L$ by $f(P_L, P_R)$, we see that $f(P_L, P_R) = (P_R - P_L)f(1, 0)$. Let $k = -f(1, 0)/\delta$. It is clear that $k > 0$ as
a consequence of the maximal-minimal principle, and \( f(P_L, P_R) = -k(P_R - P_L)/\delta. \)

**Appendix B. Convergence of Algorithm 2.2.**

We recall the definitions of \( G, K, \) and \( A \) as in (2.20)-(2.21). First we show if the scheme is convergent, it converges to a solution of (2.6).

**Lemma B.1.** If \( P^{(n)} \) converges to \( P^* = [P_1^*, P_2^*, ..., P_N^*]^T \) as \( n \) tends to infinity, then \( P_1^*, P_2^*, ..., P_N^* \) solve equation (2.6).

**Proof.** By substituting \( K^{(n)} \) in (2.14) into the linear equation \( K^{(n)}P^{(n+1)} = \Delta x^2 h^{(n)} \), we have

\[
\left( \frac{F_{l+\frac{1}{2}}^{(n)}}{D + P_{l}^{(n)}} \right) D^+ P_{l}^{(n+1)} - \left( \frac{F_{l-\frac{1}{2}}^{(n)}}{D + P_{l-1}^{(n)}} \right) D^+ P_{l-1}^{(n+1)} = Q_l \Delta x
\]

By taking the limit, we have \( F^*_{l+\frac{1}{2}} - F^*_{l-\frac{1}{2}} = Q_l \Delta x \) for \( l = 1, 2, ..., N \) and hence we have \( G(P^*) = 0. \)

In classical models, the conductances \( c_{ij} \) in the network model depend on geological structure only and are assumed constant in time. In this case, the proposed method is identical to the classical upscaling methods and no iteration is needed for solving \( P \).

**Lemma B.2.** Suppose the conductance \( c_{ij} \) in the network model for computing the flux \( f_{l+\frac{1}{2}} \) is independent of both macroscopic pressure \( P \) and microscopic pressure \( p \), then the macro-micro iteration scheme converges in one step. Moreover, the proposed iterative scheme coincides with the Newton’s method.

**Proof.** By Lemma A.2, the effective parameter \( K^{(n)}_{l-\frac{1}{2}} \) is independent of \( P^{(n)} \) and therefore independent of \( n \). It follows \( P^{(1)} \) and \( P^{(n)} \) satisfy the same linear system and hence \( P^{(1)} = P^{(n)} \) for all \( n \). Since \( K^{(n)}_{l-\frac{1}{2}} \) is independent of \( P^{(n)} \), it is easy to check

\[
\frac{1}{\Delta x^2} K^{(n)} = \frac{\partial G}{\partial P}(P^{(n)}),
\]

the Jacobian of \( G \) at \( P^{(n)} \), and the iteration is just Newton’s method.

**Theorem B.3.** Let \( P^* \) be a root of \( G \). Suppose there exists \( \eta > 0 \) and constants \( M \) and \( \lambda < 1 \) such that \( K_{l-\frac{1}{2}} \) are \( C^2 \) for \( l = 1, 2, ..., N \) and \( \|K^{-1}\| \leq M \), \( \|K^{-1}A\| \leq \lambda \) whenever \( \|P - P^*\| < \eta \). Then there exists \( \eta^* > 0 \) such that for initial vector \( P^{(0)} \) satisfies \( \|P^{(0)} - P^*\| < \eta^* \), the sequence \( P^{(n)} \) generated by the scheme converges to \( P^* \).

**Proof.** Since \( K_{l-\frac{1}{2}} \) are \( C^2 \) for \( l = 1, 2, ..., N \) for \( \|P - P^*\| < \eta \), Taylor expansion of \( G \) at \( P \) is

\[
0 = G(P^*) = G(P) + J(P)(P^* - P) + R(P),
\]

where \( J \) is the Jacobian of \( G \), and the remainder \( R(P) \) satisfies \( \|R(P)\| \leq R_1 \|P - P^*\|^2 \) for some constant \( R_1 \). Therefore, for \( \|P^{(n)} - P^*\| < \eta \)

\[
G(P^{(n)}) = -J(P^{(n)})(P^* - P^{(n)}) - R(P^{(n)})
\]

Combining with (2.20) leads to

\[
P^{(n+1)} = P^{(n)} - \left( \frac{1}{\Delta x^2} K^{(n)} \right)^{-1} G(P^{(n)}) = P^* + K^{-1} A(P^{(n)})(P^* - P^{(n)}) + \Delta x^2 K^{-1} R(P^{(n)})
\]
Let $R_2 = MR_1 \Delta x^2$ and $\eta^* = \min\{\eta_1, (1 - \lambda)/(2R_2)\}$. Assume $\|P^{(n)} - P^*\| < \eta^*$, then we have

$$\|P^{(n+1)} - P^*\| \leq \lambda\|P^{(n)} - P^*\| + R_2\|P^{(n)} - P^*\|^2 \leq \left(1 + \frac{\lambda}{2}\right)\|P^{(n)} - P^*\| < \eta^*$$

Hence by induction, if $\|P^{(0)} - P^*\| < \eta^*$,

$$\|P^{(n)} - P^*\| \leq \left(1 + \frac{\lambda}{2}\right)^n\|P^{(0)} - P^*\| < \left(1 + \frac{\lambda}{2}\right)^n\eta^*$$

which converges to 0.

**Appendix C. Error Analysis for the Elliptic Homogenization Case.** In this section, we investigate the error between the microscopic pressure and macroscopic pressure computed by our method. Our observation is that equation (2.1) can be interpreted as a discretization of an elliptic problem under some assumption on the network configuration. For such systems, we can estimate the accuracy of our proposed multiscale method via (numerical) homogenization theory.

For simplification, we only demonstrate two dimensional case, but the argument works for higher dimensional cases also. Let $\Omega = [x_L, x_R] \times [y_B, y_T]$ be a rectangular domain. Consider the following elliptic equation

$$-\nabla \cdot (a(x) \nabla p_\epsilon(x)) = 0, \quad x \in \Omega; \quad p_\epsilon(x) = g(x), \quad x \in \partial\Omega; \quad (C.1)$$

where $a_\epsilon(x) := a(x, x/\epsilon)$ for some positive smooth function $a(x, y)$ that is periodic in $y$ with period 1 in first and second coordinates for any fixed $x$, and $g$ is the given Dirichlet boundary condition. The parameter $\epsilon$ is a small positive number that refers to the length scale of rapid oscillation of coefficient. We divide the domain into $n \times m$ partitions and let $\delta x = (x_R - x_L)/n, x_i = x_L + i \delta x$ and $\delta y = (y_T - y_B)/m, y_j = y_B + j \delta y$, where $n$ and $m$ are chosen large enough to resolve $\epsilon$ scale. Let $x_{i,j} = (x_i, y_j)$. We discretize (C.1) by

$$-a_\epsilon(x_{i+\frac{1}{2}, j}) \frac{p_{i+1,j} - p_{i,j}}{\delta x} + a_\epsilon(x_{i-\frac{1}{2}, j}) \frac{p_{i,j} - p_{i-1,j}}{\delta x} - a_\epsilon(x_{i,j+\frac{1}{2}}) \frac{p_{i,j+1} - p_{i,j}}{\delta y} + a_\epsilon(x_{i,j-\frac{1}{2}}) \frac{p_{i,j} - p_{i,j-1}}{\delta y} = 0$$

where $x_{i+\frac{1}{2}, j}$ is the middle point (quadrature point) of $x_{i,j}, x_{i+1,j}$ and $p_{i,j}$ is the nodal value of the finite element solution to approximate $p_\epsilon(x_{i,j})$. By standard convergence theory, we have

$$\|p_{i,j} - p_\epsilon(x_{i,j})\| < C_1(\epsilon, a)h^2, \quad (C.3)$$

where $h = \max\{\delta x, \delta y\}$ and $C_1(\epsilon, a)$ is a constant independent of $h$ but may depend on $\epsilon, a$ and boundary value $g$.

On the other hand, the discrete system defined in (C.2) can be viewed as equations of conservation law of a linear network model for pressures $p_{i,j}$ pores; see equation (2.1): the graph of the network model is simply square lattice grids and each pore connects to four adjacent pores. The conductance $c_{i+\frac{1}{2}, j}$ of the throat connecting pore $(i, j)$ and pore $(i+1, j)$ is given by

$$c_{i+\frac{1}{2}, j} = a_\epsilon(x_{i+\frac{1}{2}, j})/\delta x,$$
and conductance $c_{i,j+\frac{1}{2}}$ of the throat connecting pore $(i, j)$ and pore $(i, j+1)$ is defined analogously.

Suppose we apply the macroscopic 2D model and macro-micro algorithm to this network model. Then the macroscopic pressure $P$ satisfies

$$\nabla \cdot (\bar{A}(x) \nabla P) = 0, \quad x \in \Omega; \quad \bar{P}(x) = g(x), \quad x \in \partial \Omega \quad (C.5)$$

where $\bar{A}$ is the homogenized coefficient which can be obtained by solving a cell problem (See [11] for more detail). Then standard homogenization theory has that

$$||\bar{P} - p_\epsilon||_\infty < C_2(a)\epsilon, \quad (C.6)$$

where the constant $C_2$ depends on $a$ only.

Notice that $\bar{A}$ can be a non-diagonal $2 \times 2$ matrix even $a$ is a scalar. We use $\bar{A}^{i,j}$ to denote which the $(i, j)$ entry of $\bar{A}$. The homogenized equation can be discretized by

$$\begin{align*}
-\bar{A}^{1,1}(y_{k+\frac{1}{2},l})D_+^{x} \bar{P}_{k,l} &+ \bar{A}^{1,1}(y_{k-\frac{1}{2},l})D_-^{x} \bar{P}_{k,l} - \bar{A}^{2,2}(y_{k,l+\frac{1}{2}})D_+^{y} \bar{P}_{k,l} \\
+ \bar{A}^{2,1}(y_{k,l+\frac{1}{2}})D_-^{y} \bar{P}_{k,l} &+ \bar{A}^{2,1}(y_{k,l-\frac{1}{2}})D_0^{y} \bar{P}_{k,l} + \bar{A}^{2,1}(y_{k,l-\frac{1}{2}})D_0^{y} \bar{P}_{k,l+\frac{1}{2}} = 0 \\
-\bar{A}^{2,1}(y_{k,l+\frac{1}{2}})D_0^{y} \bar{P}_{k,l+\frac{1}{2}} &+ \bar{A}^{2,1}(y_{k,l-\frac{1}{2}})D_0^{y} \bar{P}_{k,l-\frac{1}{2}} = 0
\end{align*} \quad (C.7)$$

where $y_{k,l} = (x_L + k \Delta x, y_B + l \Delta y)$ and $y_{l+\frac{1}{2}}$ is the middle point (quadrature point) of $y_{k,l}$ and $y_{k+1,l}$. Again, we have the estimate

$$||\bar{P}_{k,l} - \bar{P}(y_{k,l})|| < C_3(a)H^2, \quad (C.8)$$

where $H = \max \{\Delta x, \Delta y\}$ and $C_3$ is independent of $H$. We observe that $\bar{P}_{k,l}$ and $P_{k,l}$ satisfy similar equations (C.4) and (C.7). If we can estimate the difference between coefficients in (C.4) and (C.7), then we have error estimate between $\bar{P}_{k,l}$ and $P_{k,l}$.

Let $V$ be a piecewise linear function on $B_\delta(y_{k+\frac{1}{2},l})$ that is a square centered at the quadrature point $y_{k+\frac{1}{2},l}$ with length $\delta$. For each linear function $V$ and $B_\delta(y_{k+\frac{1}{2},l})$, let $v_\epsilon$ be the solution of

$$\begin{align*}
-\nabla \cdot (a(x) \nabla v_\epsilon(x)) &= 0, \quad x \in B_\delta(y_{l+\frac{1}{2}}) \\
v_\epsilon(x) &= V(x), \quad x \in \partial B_\delta(y_{l+\frac{1}{2}})
\end{align*} \quad (C.9)$$

The HMM method [25] suggests to estimate the homogenized coefficient $\bar{A}$ at quadrature point by $A_H$, which is defined as

$$\nabla W A_H(y_{k+\frac{1}{2},l}) \nabla V = \frac{1}{\delta^2} \int_{B_\delta(y_{k+\frac{1}{2},l})} \nabla w_\epsilon(x) a(x) \nabla v_\epsilon(x) \, dx,$$
where \( v_r \) and \( w_r \) are solutions of (C.9) associated with \( V \) and \( W \) respectively. Notice that (C.9) implies
\[
\int_{B_\delta(y_k+\frac{1}{2},l)} \nabla(w_r(x) - W) a_r(x) \nabla v_r(x) \, dx = 0
\]

Therefore we have
\[
\nabla W A_H(y_k+\frac{1}{2},l) \nabla V = \nabla W \left( \frac{1}{\delta x} \int_{B_\delta(y_k+\frac{1}{2},l)} a_r(x) \nabla v_r(x) \, dx \right) = \nabla W \cdot F(\nabla V),
\]
where \( F(\nabla V) \) is the average of \( a_r(x) \nabla v_r(x) \) on \( B_\delta \).

On the other hand, the local network solution \( p_{k,j} \) for computing local flux \( \hat{f} \) in our scheme is exactly the discrete solution of (C.9) using grid size \( \delta x \) and \( \delta y \) with boundary condition given by linear interpolation of a linear function obtained from \( P_{k,l}, P_{k+l,1}, P_{k+l,-1}, P_{k+1,l}, P_{k+1,l-1} \). And our local flux \( \hat{f} \) is mean value of discrete flux in each throats. Since the discretization has second order accuracy in pressure, we have first order accuracy in flux and also its mean value:
\[
\| F(\nabla P) - \hat{f} \| \leq C_1 h.
\]
By choosing \( \nabla W \) to be \([1, 0]^T \) and \([0, 1]^T \) and using the definition of \( K \)'s in our algorithm with the above flux estimate, we get
\[
|A_{1,m}^H(y_k+\frac{1}{2},l) - K_{k,\frac{1}{2},l}^1| \leq C_1 h, \quad |A_{2,m}^H(y_k,\frac{1}{2},l) - K_{k,\frac{1}{2},l}^2| \leq C_1 h
\]
for \( m = 1, 2 \). By triangle inequality, we obtain the error between coefficients:
\[
|K_{k+\frac{1}{2},l} - \bar{A}(y_k+\frac{1}{2},l)| \leq |K_{l+\frac{1}{2}}^1 - A_{1,m}^H(y_l+\frac{1}{2},l)| + |A_{1,m}^H(y_l+\frac{1}{2},l) - \bar{A}_{1,m}^H(y_l+\frac{1}{2},l)| \leq C_1 h + e(HMM),
\]
where \( e(HMM) = \| A_H(y_k+\frac{1}{2},l) - \bar{A}(y_k+\frac{1}{2},l) \| \). Combining (C.4), (C.7) and (C.10), it leads to
\[
\| T_{k,l} - P_{k,l} \| \leq C_5(e(HMM) + h) \quad \text{(C.11)}
\]
Denote \( i_k, j_l \) the indices such that \( x_{i_k,j_l} = y_{k,l} \), for each \( k \) and \( l \). Using (C.3), (C.8), (C.6) and (C.11), we obtain the final estimate
\[
\| P_{k,l} - p_{i_k,j_l} \| \leq \| P_{k,l} - T_{k,l} \| + \| T_{k,l} - T(y_{k,l}) \| + \| T(y_{k,l}) - p_r(y_{k,l}) \| + \| p_r(y_{k,l}) - p_{i_k,j_l} \| < C_1(e, a) h + C_6(a)(H^2 + e + e(HMM)),
\]
\[\text{(C.12)}\]
Recall that the HMM error \( e(HMM) \) can be controlled by
\[
e(HMM) \leq \left\{ \begin{array}{ll}
C_4 \epsilon, & \text{if } \delta = \epsilon \\
C_4(\delta + \epsilon/\delta), & \text{else}
\end{array} \right. \quad \text{\text{(C.13)}}
\]
See [28] for more reference. Summarizing above discussion, we have proved
Theorem C.1. Given a 2D linear network model whose graph is simply a lattice grids, and each pores connect to adjacent four pores. Suppose the conductance $c_{i+\frac{1}{2},j}$ of the throat connecting pore $(i, j)$ and pore $(i+1, j)$ is given by

$$c_{i+\frac{1}{2},j} = a(x_{i+\frac{1}{2},j})/\delta x,$$

and the conductance $c_{i,j+\frac{1}{2}}$ of the throat connecting pore $(i, j)$ and pore $(i, j+1)$ is given by

$$c_{i,j+\frac{1}{2}} = a(x_{i,j+\frac{1}{2}})/\delta x,$$

where $a(x) = a(x, x/\epsilon)$ for some continuous $a(x, y)$ and $a$ is periodic function in $y$ with period 1. Let $p_{i,j}$ be the pressure of the network model and $P_{k,l}$ is the macroscopic pressure computed from macro-micro algorithm with sampling size $\delta$. Let $i_k, j_l$ denote the index such that $p_{i_k,j_l}$ and $P_{k,l}$ are at the same point. Then there exists constants $C$ and $D$ such that

$$\|P_{k,l} - p_{i_k,j_l}\| < C(\epsilon, a)h + D(a)(H^2 + \epsilon^2),$$

where $C$ depends on $\epsilon$ and $a$, and $D$ depends on $\epsilon$ only.

Appendix D. Comparison to other common nonlinear solvers.

Below, we present an example which demonstrates the efficiency of our proposed method as a solver for nonlinear equations. To do this, we ignore the additional difficulties that may be caused by items 2 and 3 listed above by assuming that the analytical form of the macro flux is known and that the values of the flux can be evaluated without any errors. We compare the performance of the proposed scheme to two classical iterative root finding schemes: Newton’s method and Broyden’s method [15].

Experiment 7. (Comparison of different nonlinear solvers for computing macro pressure) Consider the flux function

$$F(P_{l-1}, P_l) = -\left(\frac{P_{l-1} + P_l}{2}\right) D^+ P_{l-1} = \frac{P_{l-1}^2 - P_l^2}{2\Delta x}, \quad \text{for} \quad l = 1, 2, \ldots, N.$$ We look for the solution $\{P_l\}_{l=0}^N$ of the equation

$$F(P_{l-1}, P_l) = F(P_l, P_{l+1}), \quad \text{for} \quad l = 1, 2, \ldots, N,$$

with the boundary conditions $P_0 = 1$ and $P_N = 0$. For the given boundary condition, the exact solution is given by $P_l = \sqrt{1 - L/N}$. With $G$ is defined in (2.19), Newton’s method, the proposed method and Broyden’s method can all be arranged into the same form:

$$P^{(n+1)} = P^{(n)} - \left(M^{(n)}\right)^{-1} G(P^{(n)}),$$

but with different choices for the matrix $M^{(n)}$:

- Newton’s method: $M^{(n)} = J(P^{(n)})$, the Jacobian of $G$ at $P^{(n)}$. The Jacobian $J$ in this example is a tridiagonal matrix with $J_{l,l} = P_l/\Delta x^2$, $J_{l,l+1} = -P_{l+1}/(2\Delta x^2)$ and $J_{l+1,l} = -P_l/(2\Delta x^2)$
The proposed method: $M^{(n)} = K^{(n)}/\Delta x^2$ as described in (2.17). The $K$ in this example is tridiagonal with $K_{l,l} = (P_{l-1} + 2P_l + P_{l+1})/2$ and $K_{l,l+1} = -(P_{l+1} + P_l)/2$.

The Broyden’s method: $M^{(n)}$ is a rank-one updated matrix constructed from $M^{(n-1)}$ that satisfies

$$M^{(n)} \left( P^{(n)} - P^{(n-1)} \right) = G(P^{(n)}) - G(P^{(n-1)})$$

and

$$M^{(n)} Q = M^{(n-1)} Q, \quad \forall Q \perp \left( P^{(n)} - P^{(n-1)} \right)$$

The initial matrix $M^{(0)}$ is typically chosen to be the Jacobian of $G$ at $P^{(0)}$ or the identity matrix $I$.

We note that in general $J$ is not necessary symmetric but $K$ used in our scheme is.

The initial guess in this experiment is chosen to be $P_l^{(0)} = 1 - l/N$. The stopping criteria is that $\|G(P^{(n)})\|_\infty < 10^{-12}$. In the Broyden’s scheme we set the initial matrix $M^{(0)}$ to be either the Jacobian $J(P^{(0)})$ evaluated at the initial guess or the identity matrix $I_N$.

Figure D.1 shows that only Newton’s method and the proposed method converge to the correct solution for simulations with $N = 50$. Broyden’s method diverges for either choice of $M^{(0)}$. The plots suggest that both methods do not suffer from higher dimensionality of solution in this particular example and that the performance of our scheme is comparable to Newton’s method.

REFERENCES


