Numerical methods for wave propagation in solids containing faults and fluid-filled fractures

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**Numerical methods for wave propagation in solids containing faults
and fluid-filled fractures**

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Abstract

This thesis develops numerical methods for the simulation of wave propagation in solids containing faults and fluid-filled fractures. These techniques have applications in earthquake hazard analysis, seismic imaging of reservoirs, and volcano seismology. A central component of this work is the coupling of mechanical systems. This aspect involves the coupling of both ordinary differential equations (ODE)(s) and partial differential equations (PDE)(s) along curved interfaces. All of these problems satisfy a mechanical energy balance. This mechanical energy balance is mimicked by the numerical scheme using high-order accurate difference approximations that satisfy the principle of summation by parts, and by weakly enforcing the coupling conditions.

The first part of the thesis considers the simulation of dynamic earthquake ruptures along non-planar fault geometries and the simulation of seismic wave radiation from earthquakes, when the earthquakes are idealized as point moment tensor sources. The dynamic earthquake rupture process is simulated by coupling the elastic wave equation at a fault interface to nonlinear ODEs that describe the fault mechanics. The fault geometry is complex and treated by combining structured and unstructured grid techniques. In other applications, when the earthquake source dimension is smaller than wavelengths of interest, the earthquake can be accurately described by a point moment tensor source localized at a single point. The numerical challenge is to discretize the point source with high-order accuracy and without producing spurious oscillations.

The second part of the thesis presents a numerical method for wave propagation in and around fluid-filled fractures. This problem requires the coupling of the elastic wave equation to a fluid inside curved and branching fractures in the solid. The fluid model is a lubrication approximation that incorporates fluid inertia, compressibility, and viscosity. The fracture geometry can have local irregularities such as constrictions and tapered tips. The numerical method discretizes the fracture geometry by using curvilinear multiblock grids and applies implicit-explicit time stepping to isolate and overcome stiffness arising in the semi-discrete equations from viscous diffusion terms, fluid compressibility, and the particular enforcement of the fluid-solid coupling conditions. This numerical method is applied to study the interaction of waves in a fracture-conduit system. A methodology to constrain fracture geometry for oil and gas (hydraulic fracturing) and volcano seismology applications is proposed.

The third part of the thesis extends the summation-by-parts methodology to staggered grids. This extension reduces numerical dispersion and enables the

formulation of stable and high-order accurate multiblock discretizations for wave equations in first order form on staggered grids. Finally, the summation-by-parts methodology on staggered grids is further extended to second derivatives and used for the treatment of coordinate singularities in axisymmetric wave propagation.

Sammanfattning på svenska

I denna avhandling utvecklas beräkningsmetoder för simulering av vågutbredning i elastiska kroppar med förkastningar och vätskefyllda sprickor. Teknikerna som utvecklas har tillämpningar inom riskbedömning av jordbävningar, seismisk bildanalys av reservoarer och vulkanseismologi. En central komponent i avhandlingen är kopplingar av mekaniska system. Med detta så avses kopplingar av ordinära differential ekvationer (ODE):er och partiella differential ekvationer (PDE):er längs med krökta gränssytor. Alla problem som behandlas uppfyller en mekanisk energibalans. Denna energibalans imiteras av det numeriska schemat genom användning av högre ordningens differensapproximationer som uppfyller partiell summation (summation-by-parts), och genom att sätta kopplingsvillkoren svagt.

Den första delen av avhandlingen behandlar simulering av dynamiska jordbävningssfenomen längs med icke-plana förkastningsgeometrier och simulering av seismisk vågutbredning från jordbävningar, när jordbävningarna är idealiserade som punktkällor. Den dynamiska jordbävningsprocessen simuleras genom att koppla den elastiska vågekvationen längs med en förkastningslinje till icke-linjära ODE:er som beskriver förkastningslinjens mekanik. Förkastningsgeometrin är komplex och behandlas genom att kombinera strukturerade och ostrukturerade nättekniker. I andra tillämpningar, när källdimensionerna hos en jordbävning är mindre än en våglängd av intresse, så kan jordbävningen noggrant beskrivas av en punktkälla. Den numeriska utmaningen är att diskretisera punktkällan med hög noggrannhetsordning utan att producera falska störningar.

Den andra delen av avhandlingen presenterar en numerisk method för vågutbredning i och runt omkring vätskefyllda sprickor. Detta problem kräver att den elastiska vågekvationen kopplas till en vätska inuti krökta och förgrenande sprickor inneslutna i en elastisk kropp. Vätskemodellen ges av en approximation som tar hänsyn till tröghet, kompressibilitet, och viskositet. Sprickgeometrin kan ha lokala ojämnheter såsom avsmalningar och spetsiga sprickändar. Den numeriska metoden approximerar sprickgeometrin genom att använda kurvlinjära multi-blocknät och tillämpar en implicit-explicit tidsstegning för att kringgå styvhet som uppstår i det semi-diskreta fallet på grund av viskosa diffusionstermer, vätskekompressibilitet, och i kopplingen. Denna numeriska metod är tillämpad för att studera interaktionen av vågor i en ledning kopplad till sprickor. En teknik för att kartlägga sprickgeometri i hydraulisk spräckning och vulkanseismologi föreslås.

Den tredje delen av avhandlingen utökar summation-by-parts tekniken till nät

med olika noder för olika delar av lösningen (staggered grids). Denna utökning möjliggör formuleringar av stabila och högre ordningens multiblockdiskretiseringar av vågekvationer på första ordningens form med förbättrade dispersionsegenskaper. Till sist så utvecklas summation-by-parts-teknologin på staggered grids till andra derivator och används för att behandla koordinat-singulariteter i axisymmetrisk vågutbredning.

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List of Papers

This thesis is based on the following papers, which will be referred to in the text by their roman numerals.

- I.** O. O'Reilly, J. Nordström, J. E. Kozdon, and E. M. Dunham, Simulation of Earthquake Rupture Dynamics in Complex Geometries Using Coupled Finite Difference and Finite Volume Methods, *Communications in Computational Physics*, (2015), 17, 2, 532–555
- II.** N. A. Petersson, O. O'Reilly, B. Sjögreen, and S. Bydlon, Discretizing singular point sources in hyperbolic wave propagation problems *Journal of Computational Physics*, (2016), 321, 532–555
- III.** O. O'Reilly, E.M. Dunham, and J. Nordström, Simulation of wave propagation along fluid-filled cracks using high-order summation-by-parts operators and implicit-explicit time stepping, Submitted (2016)
- IV.** C. Liang, O. O'Reilly, E. M. Dunham, and D. Moos, Hydraulic fracture diagnostics from Krauklis wave resonance and tube wave reflections, In review (2016)
- V.** O. O'Reilly, T. Lundquist, J. Nordström, E. M. Dunham, Energy stable and high-order accurate finite difference methods on staggered grids, In preparation
- VI.** B. Prochnow, O. O'Reilly, E. M. Dunham, and N. A. Petersson, Treatment of the polar coordinate singularity in axisymmetric wave propagation using high-order summation-by-parts operators on a staggered grid, In review (2016)

I wrote the papers I, III, and V. For these papers, I also did the software implementation that was used to produce the numerical results. My advisers J. Nordström and E. M. Dunham assisted me in the process by providing generous feedback and editorial support.

I worked on Paper II together with N. A. Petersson. We developed the theory, with the exception of the proof of convergence which was derived by B. Sjögreen.

I performed the one-dimensional numerical computations and I also assisted S. Bydlon with the 3D elastic wave computations.

Paper IV was co-written by C. Liang and E. M. Dunham. I assisted C. Liang with the numerical computations that were used to produce many of the results. I also made theoretical contributions.

Paper VI was written by B. Prochnow, a co-term master's student supervised by E. M. Dunham. I contributed to the numerical sections of the paper and assisted B. Prochnow with the implementation and production of the numerical results. In particular, I developed the theory and the construction of the operators. I also developed the test code that was included in the supplementary material.

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Introduction

Many natural and engineered systems involve elastic solids containing discontinuities such as faults and fractures. Earth's brittle crust contains faults that host earthquake ruptures. Oil and gas reservoirs, as well as aquifers and enhanced geothermal systems, also contain faults and fluid-filled fractures. In many cases these are engineered hydraulic fractures that are introduced to alter the reservoir permeability and to thereby facilitate production and flow. Glaciers and ice sheets contain fluid-filled fractures in the form of water-filled crevasses or thin layers of water at the glacier bed. Fluid-filled fractures are also found in volcanoes as magma-filled dikes and sills.

A common feature of these systems is the important role played by seismic waves. Earthquakes are natural sources of seismic waves, and it is essential for hazard purposes to understand the earthquake rupture process and the shaking carried by radiated seismic waves. In other contexts, waves are used to place constraints on the location and geometry of fractures. In oil and gas applications, the interaction of waves in the wellbore coupled to fractures may be used to constrain fracture geometry. This information could enhance reservoir production in many ways, by for example, improving the delivery of proppant, and detection of constrictions in fractures. At active volcanoes, propagation of acoustic gravity waves in magma-filled conduits connected to dikes and sills at depth could be used to infer quantities such as gas exsolution depth and volatile content.

This thesis focuses on numerical simulation and methods development for wave propagation in these systems. The computational challenges include: the coupling of highly nonlinear ODEs to PDEs and fluid-solid coupling along curved interfaces, treatment of complex geometry, and minimization of dispersion errors. To simulate dynamic earthquake ruptures, the elastic wave equation must be coupled along non-planar interfaces. Across the interface, the tangential component of the particle velocity is field is continuous and the shear tractions are coupled to friction laws described by nonlinear ODEs. The interaction of elastic waves with fluid-filled fractures requires the coupling of the elastic wave equation to a compressible and viscous fluid. Coupling conditions such as solid-fault and fluid-solid coupling conditions are derived and enforced by applying first principles. The derivation of a mechanical energy balance is used as the central tool for analysis. For stability of the numerical scheme, it is essential to mimic

the mechanical energy balance. This is accomplished by applying difference approximations that satisfy the principle of summation by parts. This technique mimics integrations by parts and results in a discrete energy balance when the coupling conditions are weakly enforced. The application of the summation-by-parts methodology is commonly done by discretizing the governing PDEs on collocated grids. For wave equations posed in first order formulation, use of collocated grids results in a scheme with suboptimal dispersion properties. By extending the summation-by-parts methodology to staggered grids, we improve the dispersion properties of the scheme while maintaining many of the benefits with this methodology. Summation-by-parts difference operators that are constructed on a staggered grid also enables us to treat problems with coordinate singularities.

This thesis is organized in the following manner.

Chapter 2-3 provides an overview of the summation-by-parts methodology, introduces new contributions in computational mathematics, and demonstrates their application to two model problems. These model problems involve the coupling of faults and friction laws to simulate earthquake rupture dynamics and fluid-solid coupling in one dimension.

Paper I considers the problem of earthquake ruptures in complex geometries, such as around the margins of a volcanic plug. This requires the introduction of an unstructured mesh to treat the complex geometry. To retain the computational efficiency and accuracy for wave propagation away from the source region, we couple the unstructured grid to a multi-block high-order finite difference method.

Paper II continues the study of earthquakes and seismic waves, but in this case in the context of point source descriptions of the earthquake source. The goal is to discretize point sources (involving Dirac delta functions) with high-order accuracy such that the source can be placed anywhere on the grid (not necessarily on a grid point). The major numerical challenge is how to perform the discretization without triggering high frequency modes.

Paper III shifts the focus away from earthquakes to wave propagation in and around fluid-filled fractures. This problem involves the coupling of a compressible, viscous fluid contained inside curved and branching fractures to an elastic solid. The major numerical challenge that arises is how to develop a numerical method that allows fully explicit time stepping of the solid without taking a prohibitively small time step due to the presence of narrow fractures.

Paper IV presents an application of the numerical method developed in Chapter 4 featuring the interaction of waves in a wellbore-fracture system. This application investigates the possibility of detecting and inferring crack geometry using tube waves that can be excited and measured in the wellbore or at the wellhead.

Paper V revisits numerical methods for wave propagation. Many numerical methods in seismology use staggered grids due to their excellent dispersion

properties. In these methods, the enforcement of boundary conditions is challenging, especially since high-order accuracy is needed. To treat such problems, we extend the summation-by-parts methodology to staggered grids.

Finally, paper VI continues the development of the summation-by-parts staggered grid method to solve problems with second derivatives and coordinate singularities. This type of coordinate singularity arises in the discretization of the radial component of the Laplacian in cylindrical coordinates. This work was specifically motivated by interest in accounting for viscous dissipation of acoustic-gravity waves within volcanic conduits.

Summation-by-parts difference operators

In this chapter, we present summation-by-parts (SBP) difference operators for initial boundary value problems. Summation-by-parts difference operators [4, 6, 5, 7] provide a systematic procedure for constructing stable, high-order finite difference approximations of well-posed problems. Roughly speaking, an initial boundary value problem is well posed if (i) a solution exists, (ii) the solution is unique, and (iii) the solution depends continuously on the initial and boundary data. The requirement (iii) can be satisfied by deriving an energy estimate. For linear problems, (ii) follows directly from (iii) and (i) is guaranteed by choosing the correct, minimal number of boundary conditions.

For many problems in science and engineering, the derivation of an energy estimate is accomplished by applying integration by parts and enforcing the correct number and form of boundary conditions. This procedure is known as the energy method [2]. Numerical schemes that are constructed using SBP difference operators satisfy the principle of summation by parts, which mimics integration by parts. Together with a careful enforcement of the boundary conditions, the summation-by-parts property enables one to derive an energy estimate for the discrete approximation, and thus proving stability.

We begin by introducing the L_2 inner product

$$\langle u, v \rangle = \int_0^1 uv dx, \quad (2.1)$$

for smooth functions $u(x, t)$ and $v(x, t)$. From calculus, we have the integration by parts formula

$$\left\langle u, \frac{\partial v}{\partial x} \right\rangle = - \left\langle \frac{\partial u}{\partial x}, v \right\rangle + u(1, t)v(1, t) - u(0, t)v(0, t). \quad (2.2)$$

Any difference operator that mimics this formula in the discrete case is an SBP operator. We shall present two ways in which SBP operators can be constructed. The first approach is a standard approach that uses a collocated grid (i.e., u and v are stored at the same grid points in a grid). The second approach uses staggered grids (i.e., u and v are stored on different grids).

2.1 SBP operators on collocated grids

We discretize the interval $x \in [0, 1]$ using $N + 1$ equidistantly spaced grid points

$$x_j = jh, \quad 0 \leq j \leq N, \quad (2.3)$$

where $h = 1/N$ is the grid spacing. We also introduce the grid functions $u(x_j, t) = u_j(t)$ and $v(x_j, t) = v_j(t)$. For convenience, we introduce the standard basis e_j of unit vectors to select specific components of a grid function. The vector e_j can be seen as a restriction operator and it is zero for all components except the j^{th} component, which is equal to 1. We have

$$u_j = e_j^T u.$$

The inner product (2.1) is approximated by the discrete inner product

$$\langle u, v \rangle_h = u^T H v,$$

where the matrix $H > 0$ is diagonal.

Next, we approximate the first derivative $\partial u / \partial x$ by the difference approximation Du , where $D = H^{-1}Q$. Each row of the matrix D contains a difference approximation. The difference approximations are $2s$ -order accurate for points in the interior and s -order accurate for points near the boundary. We refer to the order of accuracy of an SBP operator by its interior order of accuracy. In the interior a central finite difference approximation is used and on the boundary a one-sided difference approximation is used. For example, second-order accuracy in the interior is given by

$$\left. \frac{\partial u}{\partial x} \right|_{x=x_j} = \frac{u_{j-1} - u_{j+1}}{2h} + \mathcal{O}(h^2). \quad (2.4)$$

To mimic integration by parts, the matrix Q satisfies the SBP property

$$Q + Q^T = e_N e_N^T - e_0 e_0^T = \text{diag}([-1, 0, \dots, 0, 1]). \quad (2.5)$$

Using this property, we arrive at the summation-by-parts formula

$$\langle u, Dv \rangle_h = -\langle Du, v \rangle_h + u_N v_N - u_0 v_0, \quad (2.6)$$

which mimics the integration by parts formula (2.2).

The following is an example of a second-order accurate SBP operator.

$$Q = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} \\ & & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad H = \text{diag} \left(\left[\frac{1}{2}, 1, 1, \dots, 1, \frac{1}{2} \right] \right) h.$$

High-order SBP operators are constructed by applying the same principles, but with more complicated boundary closures. The use of a diagonal matrix H is not necessary, and one can improve the accuracy of the SBP operator if H contains non-diagonal blocks at the boundaries. However, for problems with variable coefficients or in curvilinear coordinates, stability cannot be guaranteed when using block diagonal H . Since both curvilinear coordinates and variable coefficients are required in this work, we shall exclusively use a diagonal H .

2.2 Discretization of singular source terms

The discretization of singular source terms arises in many areas and applications of computational physics, for example when modeling fluid-structure interaction using the immersed boundary method, and earthquakes and explosions when the wavelength of interest is large compared to the source dimension. Due to the suboptimal dispersion properties of collocated SBP operators, one needs to be careful when designing source discretizations for hyperbolic problems. Otherwise, spurious modes can be generated and destroy the accuracy of the numerical solution.

Consider the advection equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = g(t)\delta(x - x_*), \quad 0 \leq x \leq 1, \quad t \geq 0, \quad (2.7)$$

$$u(x, 0) = 0, \quad 0 \leq x \leq 1, \quad (2.8)$$

where the source time function $g(t)$ is a smooth function that satisfies $g(0) = 0$. The solution is given by

$$u(x, t) = \begin{cases} g(t - (x - x_*)), & 0 \leq x - x_* \leq t - 1 \\ 0, & \text{otherwise} \end{cases}. \quad (2.9)$$

The solution is as smooth as $g(t)$ except at $x = x_*$ if $g(t) \neq 0$.

We represent the source discretization by the vector d , which is non-zero only for $M + S$ components in a neighborhood of the source location x_* . To make d a consistent and accurate approximation, recall the definition of the Dirac distribution

$$\int_{-\infty}^{\infty} \phi(x)\delta(x - x_*)dx = \phi(x_*). \quad (2.10)$$

We approximate (2.10) by enforcing M moment conditions. The moment conditions exactly satisfy (2.10) for polynomials $\phi(x) = x^m$, $m = 0, 1, \dots, M - 1$. The moment conditions are

$$\langle d, \phi \rangle_h = x_*^s, \quad \phi_j = x_j^m, \quad m = 0, 1, \dots, M. \quad (2.11)$$

To approximate (2.7), we write

$$\frac{du}{dt} + Du = g(t)d, \quad (2.12)$$

where D is a collocated SBP operator.

The moment conditions are not sufficient for obtaining an accurate solution when using a collocated SBP operator. Consider an unresolved mode ψ (for example the Nyquist mode) and take the inner product with ψ and (2.12), which leads to

$$\frac{d\langle\psi, u\rangle_h}{dt} = -\langle\psi, Du\rangle_h + g(t)\langle\psi, d\rangle_h. \quad (2.13)$$

By the symmetry of the inner product, (2.13) can also be written as

$$\frac{d\langle\psi, u\rangle_h}{dt} = -\langle D^T\psi, u\rangle_h + g(t)\langle\psi, d\rangle_h. \quad (2.14)$$

Since the initial condition is $u(x, 0) = 0$, the spurious component is initially zero. However, the spurious component can grow in time. Suppose $D^T\psi = 0$, then we need $\langle\psi, d\rangle_h = 0$ to prevent the spurious component from growing in time. We arrive at the so-called smoothness condition

$$\langle\psi, d\rangle_h = 0. \quad (2.15)$$

To discuss the smoothness conditions in more detail, we study the periodic problem. As long as the source discretization is not near the boundary, this analysis is valid for any collocated SBP operator D in (2.12). When the source discretization is near the boundary, the analysis becomes more involved (details are omitted to save space).

In the periodic case, we can replace D with a periodic operator $\mathcal{D}$ here, which uses a centered difference approximation at each grid point. For example, a second order accurate approximation is

$$\mathcal{D}u = \frac{1}{2h} \begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 0 & 1 \\ 1 & & & -1 & 0 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix}, \quad (2.16)$$

where $u_0 = u_N$.

Since the grid function u is periodic, we can represent it using the Fourier series

$$u_j = \sum_{k=-N/2}^{N/2} \hat{u}_k e^{2\pi i k x_j},$$

assuming that N is even. The highest frequency mode that can be represented on the grid is the Nyquist mode ψ . This mode is obtained by taking the Fourier component with $k = N/2$, which yields $\psi_j = e^{\pi i N x_j} = e^{\pi i j} = (-1)^j$. Since the difference approximation is centered, we have $\mathcal{D}\psi = 0$ for $\psi_j = (-1)^j$. This is the condition that can cause the spurious mode to grow in time, see (2.14).

To prevent this growth, we make the source discretization d orthogonal to the Nyquist mode. Thus, the first smoothness condition is

$$\langle \psi, d \rangle_h = 0, \quad \psi_j = (-1)^j.$$

Additional smoothness conditions are obtained by suppressing the second highest mode $k = N/2 - 1$. The second highest mode is $\psi_j = e^{2\pi i (N/2-1)x_j} = (-1)^j e^{-2\pi i x_j}$. We perform a Taylor expansion to obtain

$$\psi_j = (-1)^j e^{-2\pi i x_j} = (-1)^j \left(1 - 2\pi i x_j + \frac{1}{2} (2\pi i x_j)^2 + \dots \right).$$

By making d orthogonal to S of the terms in the Taylor expansion, we obtain the smoothness conditions

$$\langle \psi, d \rangle_h = 0, \quad \psi_j = (-1)^j x_j^s, \quad s = 0, 1, 2, \dots, S-1. \quad (2.17)$$

In conclusion, a high-order accurate source discretization d is obtained by solving the $M + S$ equations (2.11) and (2.17). To ensure that numerical solution is p^{th} -order accurate, we need $p = M = S$ (not shown to save space).

2.3 SBP operators on staggered grids

We can mimic the integration by parts formula on staggered grids as well, and such an approximation has important implications for the dispersion properties of the numerical scheme. For example, when discretizing singular source terms it is not necessary to enforce smoothness conditions to obtain a high-order accurate numerical solution.

We introduce additional grid points stored half-way between the grid points x_j in (2.3)

$$x_{j-1/2} = (j - 1/2)h, \quad 1 \leq j \leq N.$$

Using these new grid points, the staggered grids are defined as

$$x_+ = [x_0, x_1, \dots, x_N]^T, \quad x_- = [x_0, x_{1/2}, \dots, x_{N-1/2}, x_N]^T.$$

Note that the grid x_+ has $N + 1$ grid points whereas the grid x_- has $N + 2$ grid points. Both grids include the boundary points x_0 and x_N . On each grid, we

define grid functions u for x_+ , and v for x_- . With a slight abuse of notation, a discrete inner product is defined for each grid,

$$\langle u, u \rangle_h = u^T H_+ u, \quad \text{and} \quad \langle v, v \rangle_h = v^T H_- v. \quad (2.18)$$

Next, we define a difference approximation on each grid. The difference approximation D_+ acts on a grid function defined on x_- , but approximates the derivative on x_+ . Similarly, the difference approximation D_- acts on a grid function defined on x_+ , but approximates its derivative on x_- .

SBP staggered grid operators are constructed by using central difference approximations in the interior, and one-sided difference approximations near the boundary. For example, second-order accuracy in the interior is given by the standard central approximation

$$\left. \frac{du}{dx} \right|_{x_{i-1/2}} \approx \frac{u_i - u_{i-1}}{h}, \quad \left. \frac{dv}{dx} \right|_{x_i} \approx \frac{v_{i+1/2} - v_{i-1/2}}{h}, \quad (2.19)$$

assuming smooth grid functions u and v defined on x_+ and x_- , respectively. These difference approximations are written as $D_+ = H_+^{-1} Q_+$ and $D_- = H_-^{-1} Q_-$, and satisfy the modified SBP property

$$Q_+ + Q_-^T = e_{N+} e_{N-}^T - e_{0+} e_{0-}^T. \quad (2.20)$$

The relation (2.20) leads to

$$\langle u, D_+ v \rangle_h = -\langle D_- u, v \rangle_h + u_N v_N - u_0 v_0, \quad (2.21)$$

where u is defined on x_+ and v is defined on x_- , which mimics the integration by parts formula (2.2).

A second order accurate pair of SBP staggered grid operators is

$$Q_+ = \begin{bmatrix} -\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & & & & \\ -\frac{1}{2} & -\frac{1}{4} & \frac{3}{4} & & & & \\ & & -1 & 1 & & & \\ & & & \ddots & \ddots & & \\ & & & & -1 & 1 & \\ & & & & -\frac{3}{4} & \frac{1}{4} & \frac{1}{2} \\ & & & & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} \end{bmatrix},$$

$$Q_- = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & & & & & \\ -\frac{1}{4} & \frac{1}{4} & & & & & \\ -\frac{1}{4} & -\frac{3}{4} & & & & & \\ & & -1 & 1 & & & \\ & & & \ddots & \ddots & & \\ & & & & -1 & 1 & \\ & & & & & & \frac{3}{4} & \frac{1}{4} \\ & & & & & & -\frac{1}{4} & \frac{1}{4} \\ & & & & & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix},$$

and

$$H_+ = \text{diag} \left(\left[\frac{1}{2}, 1, 1, \dots, 1, \frac{1}{2} \right] \right) h,$$

$$H_- = \text{diag} \left(\left[\frac{1}{2}, \frac{1}{4}, \frac{5}{4}, 1, \dots, 1, \frac{5}{4}, \frac{1}{4}, \frac{1}{2} \right] \right) h.$$

2.3.1 Second derivatives

A natural way to construct a second derivative approximation is to apply the first derivative twice, i.e. $D_2 = DD$. If collocated SBP operators are used, the spurious modes discussed in the previous section persists. This problem prevails even for parabolic problems, with dissipation. Another disadvantage with collocated operators is that the stencil width of the operator obtained by applying the first derivative twice grows. The width of the interior stencil in this discretization is $2w - 1$, where w is the width of the interior stencil of the first derivative. For collocated SBP operators, $w - 1$ is the interior order of accuracy of the SBP operator. If a compact second derivative is used, then the optimal stencil width w is obtained. For example, a fourth-order first derivative has $w = 5$ and the resulting wide second derivative has a stencil width of 9, nearly

a factor of two from the optimal width of 5. In addition, the compact SBP operators also suppress spurious modes. These two reasons make the compact SBP operators preferred in practice. However, when variable coefficients are involved, the analysis and implementation becomes significantly more complex.

An alternative option is to construct a wide discretization using staggered SBP operators. The stencil width of a staggered SBP operator is $w - 1$. The stencil width of the resulting second derivative, becomes $2w - 3$. The staggered SBP operators suppresses spurious modes. In the fourth order example presented previously, we have a stencil width of 4 for the first derivative and stencil width of 7 for the wide discretization. The advantage of these operators over the compact operators is that the analysis involving variable coefficients simplifies.

Consider the diffusion equation with variable coefficients

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right), \quad 0 \leq x \leq 1, \quad t \geq 0, \quad (2.22)$$

where $\mu(x) > 0$. Alternately, (2.22) can be written in first-order form

$$\frac{\partial u}{\partial t} = \frac{\partial \tau}{\partial x}, \quad (2.23)$$

$$\tau = \mu \frac{\partial u}{\partial x}. \quad (2.24)$$

Then, we discretize (2.23) by introducing the grid function u on x_+ , and discretize (2.24) by τ and μ on x_- . In order to formulate the semi-discrete approximation, μ is stored in a diagonal matrix, i.e. $\mu = \text{diag}([\mu_0, \mu_{1/2}, \dots, \mu_{N-1/2}, \mu_N])$. The semi-discrete approximation becomes

$$\frac{du}{dt} = D_+ \mu D_- u,$$

or

$$\begin{aligned} \frac{du}{dt} &= D_+ \tau, \\ \tau &= \mu D_- u. \end{aligned}$$

This semi-discrete approximation is not complete because it does not enforce any boundary conditions for this problem, see the next chapter.

Application problems

In this chapter, we show how to use SBP difference operators for solving two application problems. These problems are motivated by earthquake rupture dynamics and fluid-solid coupling arising in numerous science and engineering applications. Both these classes of problems are treated using the same systematic procedure. First, the continuous problem is analyzed and it is shown that the physical coupling conditions obtained from first principles result in an energy balance. Second, we mimic the energy balance by using SBP operators and a weak enforcement of the coupling conditions. In order to weakly enforce the coupling conditions, we use the simultaneous approximation term (SAT) method [1].

3.1 Earthquake rupture dynamics

In our first application problem, we model a dynamic earthquake rupture in one dimension. To solve this problem, we couple the elastic wave equation along a fault interface to a friction law.

In one dimension, the fault is a point at which two elastic blocks are in contact and sliding in opposite directions with respect to each other. The difference in velocity across the fault is the slip velocity. Initially, each block is sliding at an extremely low creeping velocity, relative to each other. At creeping velocities, the slip velocity is $\sim$ mm/year and corresponds to the rate of movement of tectonic plates. Roughly speaking, to nucleate an earthquake rupture, strength of the fault needs to be exceeded (its resistance to sliding). An earthquake rupture can artificially be initialized by decreasing the strength of the fault by introducing a gradually increasing load that pushes the fault to failure. Once failure occurs, the slip velocity abruptly transitions from the initial, creeping velocity to co-seismic velocities $\sim$ m/s. Figure 3.1 shows snapshots in time of the earthquake rupture process. The simulation was generated using the numerical scheme developed in this section. A MATLAB implementation is available at github.com/ooreilly/thesis.

Figure 3.1: Snapshots in time of the earthquake rupture process. The particle velocity on each side of the fault $x = 0$ is shown.

3.1.1 The continuous problem

Let $x = 0$ denote the fault interface, and consider the elastic wave equation on each side of the fault,

$$\begin{aligned} \rho \frac{\partial v^{(1)}}{\partial t} &= \frac{\partial \sigma^{(1)}}{\partial x}, \quad \frac{1}{G} \frac{\partial \sigma^{(1)}}{\partial t} = \frac{\partial v^{(1)}}{\partial x}, & -1 \leq x \leq 0, \\ \rho \frac{\partial v^{(2)}}{\partial t} &= \frac{\partial \sigma^{(2)}}{\partial x}, \quad \frac{1}{G} \frac{\partial \sigma^{(2)}}{\partial t} = \frac{\partial v^{(2)}}{\partial x}, & 0 \leq x \leq 1. \end{aligned} \quad (3.1)$$

In (3.1), $v^{(k)}$ are the particle velocities and $\sigma^{(k)}$ are the shear stresses for each side $k = 1, 2$. The material parameters ρ and G are the density and shear modulus. These parameters could be discontinuous across the fault, but for simplicity we treat them as constants.

The total mechanical energy in the system, given by the sum of kinetic energies and elastic strain energies for the material on each side of the fault, (per unit area) is

$$E = \frac{1}{2} \int_{-1}^0 \rho \left(v^{(1)} \right)^2 + \frac{1}{G} \left(\sigma^{(1)} \right)^2 dx + \frac{1}{2} \int_0^1 \rho \left(v^{(2)} \right)^2 + \frac{1}{G} \left(\sigma^{(2)} \right)^2 dx. \quad (3.2)$$

Equation (3.2) is differentiated in time and (3.1) is substituted into the result,

which yields

$$\frac{dE}{dt} = \int_{x=-1}^{x=0} v^{(1)} \frac{\partial \sigma^{(1)}}{\partial x} + \sigma^{(1)} \frac{\partial v^{(1)}}{\partial x} dx + \int_{x=0}^{x=1} v^{(2)} \frac{\partial \sigma^{(2)}}{\partial x} + \sigma^{(2)} \frac{\partial v^{(2)}}{\partial x} dx.$$

By applying integration by parts (2.2) and neglecting work done by traction on exterior boundaries, the work done by tractions on the fault becomes

$$\frac{dE}{dt} = \sum_{k=1}^2 [v^{(k)} \sigma^{(k)} \hat{n}^{(k)}]_{x=0} \quad (3.3)$$

where $\sigma^{(k)} n^{(k)}$ are the shear tractions (forces per unit area), and $\hat{n}^{(1)} = 1$ and $\hat{n}^{(2)} = -1$ is the outward unit normal evaluated on each side of the fault.

At the fault interface $x = 0$, the shear tractions must be balanced and coupled to a friction law that governs the mechanics of the fault. Force balance implies that the shear tractions $\sigma^{(k)} \hat{n}^{(k)}$ for $k = 1, 2$ are equal and opposite. That is,

$$\sigma^{(1)}(0, t) \hat{n}^{(1)} = -\sigma^{(2)}(0, t) \hat{n}^{(2)}. \quad (3.4)$$

The shear tractions must be balanced by the shear strength of the fault $\tau^{(k)}$, that is

$$\tau^{(k)} = \sigma^{(k)} \hat{n}^{(k)}, \quad \tau = \tau^{(1)}. \quad (3.5)$$

Across the fault, the particle velocity field is discontinuous and its jump is the so-called slip velocity

$$V = v^{(2)}(0, t) - v^{(1)}(0, t). \quad (3.6)$$

By substituting (3.4) and (3.6) into (3.3), we get

$$\frac{dE}{dt} = -V\tau.$$

The shear strength τ , which is defined with respect to side (1), is governed by the friction law

$$\tau = F(V, \Psi), \quad \frac{d\Psi}{dt} = G(V, \Psi). \quad (3.7)$$

The friction law depends on a state variable evolves according to a non-linear evolution law that captures the history of sliding observed in laboratory experiments. All friction laws satisfy $VF(V, \Psi) \geq 0$, which yields

$$\frac{dE}{dt} = -VF(V, \Psi) \leq 0.$$

The interpretation of this result is that the mechanical of energy of the system is changed by rate of work done by tractions at the fault, which dissipate energy due to friction during sliding. To be more specific: during the rupture process, energy is flowing into the fault from the surrounding elastic material. This energy is lost due to frictional heating.

3.1.2 The discrete problem

In this section, (3.1) is discretized using the staggered SBP operators presented in Chapter 2. To enforce the coupling conditions (3.4) and (3.7) at the fault, we weakly enforce the coupling conditions by adding penalty terms.

Consider the semi-discrete approximation

$$\begin{aligned}\rho \frac{\partial v^{(1)}}{\partial t} &= D_+ \sigma^{(1)} - H_+^{-1} e_{N+} (\sigma_N^{(1)} - \sigma^{*(1)}) \hat{n}^{(1)}, \\ \frac{1}{G} \frac{\partial \sigma^{(1)}}{\partial t} &= D_- v^{(1)} - H_-^{-1} e_{N-} (v_N^{(1)} - v^{*(1)}) \hat{n}^{(1)},\end{aligned}\tag{3.8}$$

for the material on left side of the fault, and

$$\begin{aligned}\rho \frac{\partial v^{(2)}}{\partial t} &= D_+ \sigma^{(2)} - H_+^{-1} e_{0+} (\sigma_0^{(2)} - \sigma^{*(2)}) \hat{n}^{(2)}, \\ \frac{1}{G} \frac{\partial \sigma^{(2)}}{\partial t} &= D_- v^{(2)} - H_-^{-1} e_{0-} (v_0^{(2)} - v^{*(2)}) \hat{n}^{(2)}.\end{aligned}\tag{3.9}$$

for the right side of the fault. Without loss of generality, the same number of grid points on each side of the fault is used. In both of the semi-discrete approximations, $v^{(k)}$ is defined on x_+ using $N + 1$ grid points, and $\sigma^{(k)}$ is defined on x_- using $N + 2$ grid points, for $k = 1, 2$. The penalty terms are restricted to the fault $x = 0$ using the restriction operators $e_{0\pm}$ and $e_{N\pm}$. The coupling conditions are weakly enforced by choosing the numerical fluxes $v^{*(k)}$ and $\sigma^{*(k)}$, which must be selected such that the correct coupling conditions are enforced and a stable numerical scheme is obtained.

Stability

The derivation of the semi-discrete energy balance is analogous to the continuous derivation presented in the previous section. To streamline the presentation, (3.8) and (3.9) are written as

$$\begin{aligned}\rho \frac{\partial v^{(k)}}{\partial t} &= D_+ \sigma^{(k)} - H_+^{-1} e_{I+}^{(k)} (\sigma_I^{(k)} - \sigma^{*(k)}) \hat{n}^{(k)}, \\ \frac{1}{G} \frac{\partial \sigma^{(k)}}{\partial t} &= D_- v^{(k)} - H_-^{-1} e_{I-}^{(k)} (v_I^{(k)} - v^{*(k)}) \hat{n}^{(k)}.\end{aligned}\tag{3.10}$$

In this formulation, the subscript I is used to denote the grid point on the fault in each grid, i.e. $x_I^{(1)} = x_N^{(1)}$ and $x_I^{(2)} = x_0^{(2)}$. The total mechanical energy (3.2) is approximated by the discrete energy

$$E_h = \frac{1}{2} \sum_{k=1}^2 \rho \left(v^{(k)} \right)^T H_+ v^{(k)} + \frac{1}{G} \left(\sigma^{(k)} \right)^T H_- \sigma^{(k)}.\tag{3.11}$$

The rate of change in the discrete mechanical energy of is

$$\begin{aligned} \frac{dE_h}{dt} &= \sum_{k=1}^2 \left(v^{(k)} \right)^T Q_+ \sigma^{(k)} + \left(\sigma^{(k)} \right)^T Q_- v^{(k)} \\ &\quad - v^{(k)} (\sigma^{(k)} - \sigma^{*(k)}) \hat{n}^{(k)} - \sigma^{(k)} (v^{(k)} - v^{*(k)}) \hat{n}^{(k)} \\ &= \sum_{k=1}^2 v_I^{(k)} \sigma_I^{(k)} \hat{n}^{(k)} - v^{(k)} (\sigma^{(k)} - \sigma^{*(k)}) \hat{n}^{(k)} - \sigma^{(k)} (v^{(k)} - v^{*(k)}) \hat{n}^{(k)} \end{aligned} \quad (3.12)$$

To arrive at (3.12), we have used (3.10), the SBP property (2.20) for staggered grids, and neglected the contributions from the exterior boundaries.

Next, the penalty terms are considered. The idea is to mimic the energy rate in (3.3) by rewriting (3.12) as

$$\frac{dE_h}{dt} = \sum_{k=1}^2 v^{*(k)} \sigma^{*(k)} \hat{n}^{(k)} - \mathcal{R}, \quad \mathcal{R} \geq 0. \quad (3.13)$$

By adding and subtracting $v^{*(k)} \sigma^{*(k)} \hat{n}^{(k)}$ to (3.12) results in

$$\frac{dE_h}{dt} = \sum_{k=1}^2 v^{*(k)} \sigma^{*(k)} \hat{n}^{(k)} - \mathcal{R}, \quad \mathcal{R} = (v_I^{(k)} - v^{*(k)}) (\sigma_I^{(k)} - \sigma^{*(k)}) \hat{n}^{(k)}. \quad (3.14)$$

This result is the same as (3.13) with the exception of $\mathcal{R}$ being indefinite. To obtain $\mathcal{R} \geq 0$, we choose the numerical fluxes such that

$$\alpha^{(k)} (v_I^{(k)} - v^{*(k)}) = (\sigma_I^{(k)} - \sigma^{*(k)}) \hat{n}^{(k)}, \quad \alpha^{(k)} \geq 0, \quad k = 1, 2, \quad (3.15)$$

which leads to

$$\frac{dE_h}{dt} = \sum_{k=1}^2 v^{*(k)} \sigma^{*(k)} \hat{n}^{(k)} - \mathcal{R}, \quad \mathcal{R} = \alpha^{(k)} (v^{(k)} - v^{*(k)})^2 \geq 0. \quad (3.16)$$

To enforce the coupling conditions (3.4) and (3.7), we choose

$$\sigma^{*(1)} \hat{n}^{(1)} = -\sigma^{*(2)} \hat{n}^{(2)}, \quad (3.17)$$

$$\tau^* = F(V^*, \Psi), \quad (3.18)$$

where $\tau^{*(k)} = \sigma^{*(k)} \hat{n}^{(k)}$, $\tau^* = \tau^{*(1)}$, and $V^* = v^{*(2)} - v^{*(1)}$, according to (3.23) and (3.6). Finally, by inserting (3.17) and (3.18) into (3.16), we get

$$\frac{dE_h}{dt} = -V^* F(V^*, \Psi) - \sum_{k=1}^2 \alpha^{(k)} (v^{(k)} - v^{*(k)})^2 \leq 0. \quad (3.19)$$

Thus, the semi-discrete approximation dissipates energy since $V^* F(V^*, \Psi) \geq 0$, and the parameters $\alpha^{(k)} \geq 0$.

The unknowns $v^{*(k)}$ and $\sigma^{*(k)}$ are determined by solving the problem given by (3.15), (3.17), and (3.18). In general, it is not possible to obtain an explicit form for $v^{*(k)}$ and $\sigma^{*(k)}$ because the problem is nonlinear. The existence of a solution is addressed by applying the implicit function theorem, see [3] for details. Nevertheless, the nonlinear problem can be stated in a simpler form. Since $\hat{n}^{(1)} = -\hat{n}^{(2)}$, it follows that $\sigma^{*(1)} = \sigma^{*(2)}$ from (3.17). By multiplying (3.18) by $\alpha^{(2)}$ for $k = 1$ and $\alpha^{(1)}$ for $k = 2$, results in

$$\frac{\alpha^{(1)}\alpha^{(2)}(V^* - V)}{\alpha^{(1)} + \alpha^{(2)}} = \frac{\alpha^{(2)}\sigma^{(1)} + \alpha^{(1)}\sigma^{(2)}}{\alpha^{(1)} + \alpha^{(2)}} + F(V^*, \Psi), \quad (3.20)$$

where $\alpha^{(1)} + \alpha^{(2)} \neq 0$. We solve this nonlinear equation to obtain a root V^* . This root is used to compute $\sigma^{*(k)} = F(V^*, \Psi)$, and then $v^{*(k)}$ are obtained from (3.15). The choice of $\alpha^{(k)}$ influences the accuracy and stiffness of the scheme. In [3], the choice $\alpha^{(k)} = \rho c$ was used. In this case, $\alpha^{(k)}$ is the shear wave impedance of the solid given by the shear wave speed $c = \sqrt{G/\rho}$.

3.2 Fluid-solid coupling

In this section, the elastic wave equation is coupled to the diffusion equation in one dimension. This problem arises in the coupling of plane shear waves to a layer of a viscous fluid with no background flow. Due to the fluid-solid coupling, narrow boundary layers can develop in the fluid.

Consider a fluid to the left and a solid to the right. Figure 3.2 shows the tangential component of the particle velocity field in the fluid and solid with respect to the fluid-solid interface. In the solid, a shear wave in the form of Gaussian wave packet is propagating to the left, towards the fluid-solid interface. This shear wave pushes the solid in the positive y -direction (tangential to the interface). When the shear wave reaches the fluid-solid interface, the fluid is dragged along with the motion of the solid due to the no-slip condition of viscous fluid. As a consequence, a narrow boundary layer develops. The width of the boundary layer depends on the frequency at which waves in the solid interact with the interface and the rate of momentum diffusion in the fluid. As the shear wave interacts with the fluid-solid interface, the particle velocity in the solid nearly doubles. This is because the fluid impedance is low compared to the solid impedance, and therefore the solid senses the fluid almost as a free-surface. A MATLAB implementation that solves this problem is available at github.com/ooreilly/thesis.

3.2.1 The continuous problem

Again, the solid is governed by the elastic wave equation for shear waves

$$\rho_s \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial x}, \quad \frac{1}{G} \frac{\partial \sigma}{\partial t} = \frac{\partial v}{\partial x}, \quad 0 \leq x \leq 1, \quad (3.21)$$

Figure 3.2: Snapshots in time showing boundary layer development due a Gaussian wave packet that interacts with the fluid-solid interface. The fluid and solid velocity is shown.

where we have denoted the solid density by ρ_s to distinguish it from the fluid density.

The fluid is governed by the diffusion equation

$$\rho_f \frac{\partial u}{\partial t} = \frac{\partial \tau}{\partial x}, \quad (3.22)$$

$$\tau = \mu \frac{\partial u}{\partial x}, \quad (3.23)$$

for $-1 \leq x \leq 0$. In (3.22), u is the fluid velocity, and τ is the viscous shear stress (not to be confused with the fault strength in the previous example). Furthermore, ρ_f is the fluid density, and μ is the dynamic viscosity.

The total mechanical energy of the fluid-solid system (per unit area) is

$$E = \frac{1}{2} \int_{-1}^0 \rho_f u^2 dx + \frac{1}{2} \int_0^1 \rho_s v^2 + \frac{1}{G} \sigma^2 dx, \quad (3.24)$$

where the terms are the kinetic energy in the fluid, kinetic energy and elastic strain energy in the solid.

If we neglect the work done on exterior boundaries, then the rate of change of

the total mechanical energy is

$$\begin{aligned} \frac{dE}{dt} &= \int_{-1}^0 u \frac{\partial \tau}{\partial x} dx + \int_0^1 v \frac{\partial \sigma}{\partial x} + \sigma \frac{\partial v}{\partial x} dx \\ &= - \int_{-1}^0 \frac{1}{\mu} \tau^2 dx + [\tau u - \sigma v]_{x=0}, \end{aligned} \quad (3.25)$$

where we have used (3.21), (3.22) and (3.23), and applied integration by parts. The interpretation is that the rate of change of the mechanical energy is given by viscous dissipation in the fluid and work done by fluid and solid tractions on the interface. The tractions at the interface must balance, and we must also satisfy the no-slip condition of a viscous fluid:

$$\tau(0, t) = \sigma(0, t), \quad u(0, t) = v(0, t). \quad (3.26)$$

By enforcing the coupling conditions, the energy balance

$$\frac{dE}{dt} = - \int_{-1}^0 \frac{1}{\mu} \tau^2 dx \leq 0 \quad (3.27)$$

is obtained.

3.2.2 The discrete problem

Next, we construct a semi-discrete approximation, by using staggered SBP operators.

A semi-discrete approximation of the solid (3.21) is

$$\begin{aligned} \rho \frac{\partial v}{\partial t} &= D_+ \sigma + H_+^{-1} e_{I+} (\sigma_I - \sigma^*), \\ \frac{1}{G} \frac{\partial \sigma}{\partial t} &= D_- v + H_-^{-1} e_{I-} (v_I - v^*). \end{aligned} \quad (3.28)$$

This approximation is the same as the one presented in (3.9). Recall that v_I and σ_I denotes the values on the interface, and v^* and σ^* shall be determined by enforcing the coupling conditions (3.26) in a stable manner.

A semi-discrete approximation of the fluid (3.22) and (3.23) in first order form is

$$\rho_f \frac{du}{dt} = D_+ \tau - H_+^{-1} e_{I+} (\tau_I - \tau^*) - \mu H_+^{-1} D_-^T e_{I-} (u_I - u^*), \quad (3.29)$$

$$\tau = \mu D_- u. \quad (3.30)$$

Note that the shear stress τ is defined on the x_- grid and the velocity u is defined on x_+ . We have added two penalty terms to the semi-discrete approximation (3.29). The first penalty term is used to enforce a Neumann condition and the second penalty term is used to enforce a Dirichlet condition.

Stability

We define the discrete mechanical energy

$$E_h = \frac{\rho_s}{2} v^T H_+ v + \frac{1}{2G} \sigma^T H_- \sigma + \frac{\rho_f}{2} u^T H_+ u, \quad (3.31)$$

which approximates (3.24). The rate of change of the mechanical energy (3.31) becomes

$$\begin{aligned} \frac{dE_h}{dt} = & u^T H_+ D_+ \tau - u_I (\tau_I - \tau^*) - \tau_I (u_I - u^*) \\ & + v^T Q_+ \sigma + \sigma^T Q_- v + v_I (\sigma_I - \sigma^*) + \sigma_I (v_I - v^*) \end{aligned}, \quad (3.32)$$

where (3.28), (3.29), and (3.30) have been used. The SBP property (2.20) for staggered grids yields

$$\begin{aligned} u^T H_+ D_+ \tau &= u^T (-Q_-^T + e_{I+} e_{I-}^T) \tau = -\frac{1}{\mu} \tau^T H_- \tau + u_I \tau_I, \\ v^T Q_+ \sigma + \sigma^T Q_- v &= -v_I \sigma_I. \end{aligned} \quad (3.33)$$

By inserting (3.33) into (3.32), results in

$$\begin{aligned} \frac{dE_h}{dt} = & -\frac{1}{\mu} \tau^T H_- \tau + u_I \tau_I - u_I (\tau_I - \tau^*) - \tau_I (u_I - u^*) \\ & - v_I \sigma_I + v_I (\sigma_I - \sigma^*) + \sigma_I (v_I - v^*) \end{aligned} \quad (3.34)$$

Next, the penalty terms are considered. By adding and subtracting $u^* \tau^*$ and $v^* \sigma^*$ from the right hand side, we get,

$$\begin{aligned} \frac{dE_h}{dt} = & -\frac{1}{\mu} \tau^T H_- \tau + (u^* \tau^* - v^* \sigma^*) - \mathcal{R}, \\ \mathcal{R} = & (u_I - u^*) (\tau_I - \tau^*) - (v_I - v^*) (\sigma_I - \sigma^*). \end{aligned} \quad (3.35)$$

To bound $\mathcal{R}$, the numerical fluxes are chosen as

$$\alpha(u_I - u^*) = \tau_I - \tau^*, \quad \text{and} \quad \beta(v_I - v^*) = -(\sigma_I - \sigma^*) \quad (3.36)$$

where the parameters $\alpha \geq 0$ and $\beta \geq 0$, and $\alpha + \beta \neq 0$. The coupling conditions (3.26) are enforced by defining

$$v^* = u^* \quad \text{and} \quad \sigma^* = \tau^*. \quad (3.37)$$

Finally, (3.35) becomes

$$\frac{dE_h}{dt} = -\frac{1}{\mu} \tau^T H_- \tau - \alpha(u_I - u^*)^2 - \beta(v_I - v^*)^2 \leq 0. \quad (3.38)$$

The mechanical energy balance (3.38) has a dissipation term that approximates the dissipation term found in (3.27), and includes additional numerical dissipation terms that vanish with grid refinement. To determine v^* , σ^* , u^* , and τ^* , we solve (3.36) and (3.37). The solution is given by

$$\begin{aligned} u^* = v^* &= \frac{1}{\alpha + \beta}(\sigma_I - \tau_I) + \frac{1}{\alpha + \beta}(\beta v_I + \alpha u_I), \\ \tau^* = \sigma^* &= \frac{\alpha\beta}{\alpha + \beta}(v_I - u_I) + \frac{1}{\alpha + \beta}(\alpha\sigma_I + \beta\tau_I). \end{aligned}$$

Again, accuracy and stiffness of the scheme (3.28)-(3.29) depends on the choice of α and β .

Included papers

Conclusions

In this thesis, we have developed numerical methods for wave propagation in solids that contain complex geometries in the form of curved and branching faults and fluid-filled fractures. The thesis is divided up into three parts that each contain new contributions to earthquake rupture dynamics, seismic imaging of reservoir and volcanic systems, and various engineering applications that involve the interaction of waves.

Our first contribution is the treatment of complex fault geometry in earthquake rupture dynamics. Since faults only make up a small part of the computational domain, we combined unstructured and structured grids to gain computational efficiency. For earthquakes that are too small to be resolved on the grid, a point source representation can be used. We introduced a new approach that enables the discretization of point sources in hyperbolic problems with high-order accuracy. This approach avoids the triggering of spurious oscillations that can otherwise destroy the accuracy.

To simulate wave propagation in and around fluid-filled fractures, we have improved upon existing approaches by presenting a numerical method that incorporates all of the necessary physics and is computationally efficient. Computational efficiency was achieved in two ways. First, we used a lubrication-type approximation of the compressible Navier-Stokes equations, and dropped any negligible terms. Second, we constructed an implicit-explicit time partitioning that overcomes the stiffness introduced by fractures, and allows the solid to be updated in a fully explicit manner using a time-step set by the CFL condition of wave propagation.

The method was used to investigate the interaction of tube waves in a wellbore connected to fractures. The simulation of waves in this coupled system is computationally efficient. Here, computational efficiency was gained by generating an offline database of fracture transfer functions from numerous two dimensional wave propagation simulations. Each simulation used a different fracture geometry and the output of these simulations was distilled into a transfer function. The transfer function is a complex quantity that contains information about the frequency-dependent wave response of the fracture (i.e., its hydraulic impedance). The coupled fracture-wellbore system has a complicated response to excitation and we showed that under certain conditions, it is possible to amplify the resonant frequencies of the crack by altering the length of the wellbore

section containing the fracture. This condition could be useful to constrain fracture geometry.

Our final contribution is a numerical method that allows for a stable and high-order accurate multiblock coupling of staggered grids. In computational seismology, high-order finite difference methods on staggered grids are widely used for their excellent dispersion properties. However, the enforcement of boundary conditions in these numerical methods can be challenging. To solve this problem, we extended the summation-by-parts methodology to staggered grids.

With the development of new, summation-by-parts difference operators on staggered grids we were able to discretize point sources without producing spurious oscillations. We were also able to handle material discontinuities with high-order accuracy by leveraging the multi-block capabilities of the summation-by-parts methodology. Finally, we developed staggered grid difference approximations of the second derivative and used these approximations to treat the coordinate singularity in the radial component of the Laplacian.

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