A Boundary Integral Equation Method for the Laplace Equation with Dynamic Boundary Conditions

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The Problem

How to solve the differential equations with dynamic boundary conditions:

$$\begin{cases} \Delta u(\mathbf{x}, t) = 0, & \mathbf{x} \in \Omega, \\ u_t(\mathbf{x}, t) + \eta \frac{\partial u(\mathbf{x}, t)}{\partial n} = 0, & on \quad \partial \Omega, \\ u(\mathbf{x}, t = 0) = g(\mathbf{x}), & on \quad \partial \Omega, \end{cases}$$

» Dynamic

The big problem.

More general PDEs with dynamic boundary conditions

$$\begin{aligned} u_t - \Delta u &= 0 & in \quad Q = (0, \infty) \times \Omega, \\ u_t &= k u_{\nu} & on \quad [0, \infty) \times \partial \Omega, \\ u(0, x) &= u_0(x) & on \quad \Omega, \end{aligned}$$

Nonlinear Cahn-Hilliard equation with dynamic BC, Navier-Stokes/Stokes with dynamic BC

The dynamic boundary condition has been used to model many physical phenomena, including the moving contact lines, electro-wetting, and the dynamic interactions of fluid with domain wall.

Energy form

 Solving the Laplace equation with dynamic boundary condition is equivalent to solving

$$\frac{d}{dt} \int_{\Omega} \frac{1}{2} |\nabla u|^2 dx = -\int_{\partial \Omega} \frac{1}{\eta} |u_t|^2 dS$$

 More complex equations can also be derived using energetic/variational methods

Potential theory based numerical method?

We consider integral equation approach using Green's function, layer and volume potentials (interactions).

Linear constant coefficient problems ? Linear variable coefficient problems ?? Nonlinear problems ??? Moving interfaces ???

Layer potentials? Moving layer potentials ??? Layer potentials + volume potentials (or FDM/FEM)? Integral operators as preconditioners ?

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Today: A Boundary Integral Equation Method for the Laplace Equation with Dynamic Boundary Conditions

How to solve differential equations with dynamic boundary conditions:

 $\begin{cases} \Delta u(\mathbf{x},t) = 0, & \mathbf{x} \in \Omega, \\ u_t(\mathbf{x},t) + \eta \frac{\partial u(\mathbf{x},t)}{\partial n} = 0, & on \quad \partial\Omega, \\ u(\mathbf{x},t=0) = g(\mathbf{x}), & on \quad \partial\Omega, \end{cases}$ -> Dynamic BC

Potential Theory (Interactions)

Green's function (potential field due to point charge)

$$\Delta u(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{y})$$
$$G(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi} \log |\mathbf{x} - \mathbf{y}|$$

Single (simple) Layer Potential (charge on boundary)

$$S_{lp}(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y}) \mathrm{d}S_{\mathbf{y}}, \quad \forall \mathbf{x} \in \Omega$$

Double Layer Potential (dipole on boundary)

$$D_{lp}(\mathbf{x}) = \int_{\Gamma} \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n_{\mathbf{y}}} \mu(\mathbf{y}) \mathrm{d}S_{\mathbf{y}}, \quad \forall \mathbf{x} \in \Omega,$$

Dimension Reduction and Boundary Integral Equation Formulation

• Using the single layer potential, the solution becomes

$$u(\mathbf{x},t) = \int_{\Gamma} G(\mathbf{x},\mathbf{y}) \rho(\mathbf{y},t) dS_{\mathbf{y}}, \quad \mathbf{y} \in \Gamma,$$
 Where

$$\begin{cases} \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \rho_t(\mathbf{y}, t) dS_{\mathbf{y}} + \eta \frac{\partial}{\partial n_{\mathbf{x}}} \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y}, t) dS_{\mathbf{y}} = 0, \\ \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y}, 0) dS_{\mathbf{y}} = u_0(\mathbf{x}). \end{cases}$$

Note that the time-dependent unknowns are **only defined on** the boundary.

Semi-discrete Boundary Integral Equation

Applying the jump conditions of the layer potentials

$$\begin{split} \int_{0}^{2\pi} G\left(\mathbf{x}, \mathbf{z}(s)\right) \rho_{t}\left(\mathbf{z}(s), t\right) |\mathbf{z}'(s)| ds &+ \frac{1}{2} \eta \rho\left(\mathbf{x}, t\right) \\ &+ \eta \int_{0}^{2\pi} \frac{\partial G(\mathbf{x}, \mathbf{z}(s))}{\partial n_{\mathbf{x}}} \rho\left(\mathbf{z}(s), t\right) |\mathbf{z}'(s)| ds = 0, \quad (\mathbf{x}, t) \in \Gamma \times (0, T], \\ \int_{0}^{2\pi} G\left(\mathbf{x}, \mathbf{z}(s)\right) \rho\left(\mathbf{z}(s), 0\right) |\mathbf{z}'(s)| ds &= u_{0}(\mathbf{x}), \quad \mathbf{x} \in \Gamma, \end{split}$$

Apply backward Euler in time

$$\int_{0}^{2\pi} G(\mathbf{x}, \mathbf{z}(s)) \frac{\rho\left(\mathbf{z}(s), t^{k+1}\right) - \rho\left(\mathbf{z}(s), t^{k}\right)}{\Delta t} |\mathbf{z}'(s)| ds + \frac{\eta}{2}\rho(\mathbf{x}, t^{k+1}) + \eta \int_{0}^{2\pi} \frac{\partial G(\mathbf{x}, \mathbf{z}(s))}{\partial n_{\mathbf{x}}} \rho(\mathbf{z}(s), t^{k+1}) |\mathbf{z}'(s)| ds = 0, \quad (\mathbf{x}, t) \in \Gamma \times (0, T].$$

Stability of the Semi-discrete Formulation

If the integral operator is evaluated analytically, the **semidiscrete formulation is numerically stable.**

The proof is based on the spectral analysis of the single layer potential operator.

$$K = -\int_0^{2\pi} \log |\mathbf{z}(v) - \mathbf{z}(s)| e^{ins} \, ds = \begin{cases} \frac{\pi}{|n|} e^{Inv}, & n \neq 0.\\ -2\pi \log(r), & n = 0. \end{cases}$$

Spatial Discretization

State of the art high order numerical quadratures for nearsingular, singular, and hyper-singular integrals include

Quadratures with end-point corrections (e.g, trapezoidal rule with a few additional point corrections)

- Kapur-Rokhlin quadrature
- Alpert quadrature

Quadratures using potential theory (+ FMM acceleration)

• Quadrature by Expansion (QBX)

Trapezoidal Rule with end-point corrections



(a) K-R

(b) Alpert

Implementations for DC: Numerical Results

 However, numerical results show that the method is UNSTABLE!!!



Analyzing the Instability – continuous case

Consider a circle with radius r – using

$$K = -\int_0^{2\pi} \log |\mathbf{z}(v) - \mathbf{z}(s)| e^{ins} \, ds = \begin{cases} \frac{\pi}{|n|} e^{Inv}, & n \neq 0.\\ -2\pi \log(r), \, n = 0. \end{cases}$$

and the solution in Fourier series

$$u(\mathbf{x},t) = \sum_{n=-\infty}^{\infty} a_n(t) (r_1/r)^{|n|} e^{Ins_i}$$

analytical solution is described by the stiff ODE system

$$a'_{n}(t) + \eta a_{n}(t) \frac{|n|}{r} = 0, \quad u_{0}(\mathbf{x}) = \sum_{n=-\infty}^{\infty} c_{n}(r_{1}/r)^{|n|} e^{Ins_{i}}$$

Solution is then $u(\mathbf{x},t) = \sum_{n=-\infty}^{\infty} c_{n}e^{-\eta \frac{|n|}{r_{1}}t} (r_{1}/r)^{|n|} e^{Ins_{i}}$

Semi-Discrete: Continuous in x, backward Euler in t

A little algebra shows that applying the backward Euler to the PDE = applying the backward Euler (BE) to the stiff ODE system in the frequency domain

$$a_n'(t) + \eta a_n(t) \frac{|n|}{r} = 0,$$

using standard ODE theory, solving the semi-discrete system using BE is numerically stable

Problem is from the spatial quadrature

Analytical result

$$K = -\int_0^{2\pi} \log |\mathbf{z}(v) - \mathbf{z}(s)| e^{ins} \, ds = \begin{cases} \frac{\pi}{|n|} e^{Inv}, & n \neq 0.\\ -2\pi \log(r), \, n = 0. \end{cases}$$

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Numerical result

After discretization, the resulting matrix is **circulant**. **Eigenvectors of circulant matrices are discretized e**^{inx}

Let's check the eigenvalues numerically.

Numerical eigenvalues of K-R





Left figure: blue means negative eigenvalues. High-frequency eigenvalues lost accuracy!

Numerical eigenvalues of Alpert quadrature

Numerically computed eigenvalues and errors



Left figure: blue means negative eigenvalues. High-frequency eigenvalues lost accuracy!

The numerical troubles

 Let's consider the original continuous PDE in the frequency domain (truncated)

$$\int_{0}^{2\pi} rG\left(\mathbf{x}, \mathbf{z}(s)\right) \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} b'_{n}(t)e^{Ins} \, ds + \frac{1}{2}\eta \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} b_{n}(t)e^{Ins} + r\eta \int_{0}^{2\pi} \frac{\partial G\left(\mathbf{x}, \mathbf{z}(s)\right)}{\partial n_{\mathbf{x}}} \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} b_{n}(t)e^{Ins} \, ds = 0.$$

Equation for each frequency

$$rb'_n(t)\int_0^{2\pi} G\left(\mathbf{x}, \mathbf{z}(s)\right)e^{Ins}ds + b_n(t)\frac{1}{2}\eta e^{Ins} = 0$$

Semi-discrete system

 The spatially discrete temporally continuous system for each eigenvector becomes

$$r\lambda_n b'_n(t) + \frac{1}{2}\eta b_n(t) = 0, n = -\frac{N}{2} + 1, \cdots, \frac{N}{2}, n \neq 0.$$

- Note that when λ_n becomes negative, then the corresponding frequency becomes unstable!!!
- Reminder: analytical λ_n

$$K = -\int_0^{2\pi} \log |\mathbf{z}(v) - \mathbf{z}(s)| e^{ins} ds =$$

$$\frac{\pi}{|n|}e^{Inv}, \qquad n \neq 0.$$
$$-2\pi \log(r), \ n = 0.$$

The Semi-discrete system is unstable!

 Unfortunately, there are negative O(10) eigenvalues after spatial discretization...



K-R quadrature errors.

$$r\lambda_n b'_n(t) + \frac{1}{2}\eta b_n(t) = 0, n = -\frac{N}{2} + 1, \cdots, \frac{N}{2}, n \neq 0.$$

- Analytical Eigenvalue $\lambda_n = \pi/|n|$
- Numerical Eigenvalue

some λ_n 's are negative, and can be as large as -10.

In dynamic simulation, the corresponding frequency error grows as 10⁻¹⁵ 10^k after marching k steps.

Lesson learned

- K-R and Alpert quadratures are great (and state-of-theart) tools for static problems.
- K-R and Alpert quadratures produces large highfrequency errors, making them unfit for dynamic simulations if applied directly ...

How to modify these numerical quadrature rules?

· Half of the eigenvalues can be trusted.



A simple solution: Filtering the highfrequency modes

 A straight-forward scheme is to filter out the high-frequency modes completely!



Results using filtered Alpert's quadrature scheme for dynamic simulations.

Applications

 We can use the tool to study problems with dynamic boundary conditions, and answer questions like:

How does the solution depend on local curvature?

Integral Equation Method

Can we derive better boundary integral formulations?

- E.g., using double layer potential?
- Using quadruple layer potential?
- Using linear combinations of different layer potential?

How about moving interfaces?

Analytical properties of moving layer potentials. This seems to be a field not so intensively studied.

f(x, y)f(y, t) dSy

Variable and nonlinear terms?

- What if there are variable or nonlinear terms in the equation?
- How to couple potential theory with existing FEM/FDM?
- How to use integral operators to produce formulations with better condition numbers?

The energy form, PDE form, and potential theory?

How can ideas from one field be applied to a different field

E.g., can ideas from fast algorithms (FMM) based on interactions (Green's function) be applied to energy minimization problems (most existing methods using iterative line search methods)?

E.g., energy stable schemes for the boundary integral equation formulations?

Interactions(potential theory)? Energy(variational formulation)? And PDEs?

"The basic mechanisms for many PDEs are different interactions between particles (e.g., the Coulomb interactions in Poisson equations, the equations of states in Navier-Stokes equations, and the assumptions for different diffusions). The nature of the interactions often gives rise to (nonlocal) integral form models. Many pure PDE forms (e.g., diffusion and transport equations) can be viewed as approximation/truncations of the nonlocal interactions, and are the results of averaging and limiting."

– Professor Chun Liu

Take home message

- Although not commonly used it is possible to apply potential theory to interface problems.
- Theoretical and numerical properties of existing tools based on potential theory to interface (dynamic) problems still need to be studied.
- Understanding the relations between different formulations may provide new powerful tools for important applications.

Summary

We presented a boundary integral equation based numerical scheme for solving PDEs with dynamic boundary conditions.

- Interface problems with dynamics boundary condition can be solved using potential theory.
- K-R and Alpert quadratures are great tools for static problems, but they need to be modified for dynamic simulations.
- With proper filtering, we developed tool that can provide accurate and stable numerical results.

谢谢! THANK YOU!

