Dual Reciprocity Boundary Element Method for Magma Ocean Simulations

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Physical Motivation

- Earth's early history is marked by a giant impact with a Mars-sized object
- This led to a substantial amount of interior melting followed by rapid crystallization of this 'magma ocean'
- How this crystallization took place and crystals settled provide insight into the planet's rate of cooling

Abstract

- Understanding how crystals settle in a magma ocean is critical for answering questions about Earth's early history
- Experiments have been performed that have given insight into this behavior
- The ability to simulate this behavior numerically is not available
- Over the course of AMSC663 and AMSC664, a numerical solver based on the Dual Reciprocity Method has been built to address this problem

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Dual Reciprocity Method

- The Dual Reciprocity Method solves partial differential equations in the form:

$$-\Delta u = \hat{b} \quad \text{in} \quad \Omega \tag{1}$$

  with Dirichlet, Neumann, or mixed boundary conditions
- The source term, $\hat{b}$ is potentially non-linear in u
- In DRM, $\hat{b}$ is referred to as the residual term

Approximation of the Residual Term

- Approximate the residual term, by a linear combination of basis functions $\hat{f}_k$

$$\hat{b} = \sum_k \beta_k \hat{f}_k \tag{2}$$

where

$$\hat{f}_k = 1 + r_k \qquad r_k = |x - x_k| \tag{3}$$

- With this basis function we can find $\hat{u}_k$ such that

$$-\Delta \hat{u}_k = \hat{f}_k \quad \text{thus} \quad \hat{u}_k = -\frac{r^2}{4} - \frac{r^3}{9} \tag{4}$$

Some Notation

- Denote the flux density as:

$$q = \nu \cdot \nabla u \tag{5}$$

where ν is the outward facing normal vector

- Define the fundamental solution u_i^* to the Poisson in $\mathbb{R}^2$:

$$\Delta u_i^* = -\delta(x - x_i) \quad \text{so} \quad u_i^* = -\frac{1}{2\pi}\ln(r_i) \tag{6}$$

Integration by Parts: LHS

- After multiplying the general DRM PDE by the fundamental solution and integrating over the domain, use integration by parts twice:

$$\int_\Omega -\Delta u u_i^* = \int_\Gamma -q u_i^* + \int_\Gamma \nabla u \cdot \nabla u_i^* \quad (7)$$

$$= \int_\Gamma -q u_i^* + u q_i^* - \int_\Omega \Delta u_i^* u \quad (8)$$

$$= \int_\Gamma u q_i^* - q u_i^* + c(x_i) u(x_i) \quad (9)$$

- $c(x_i)$ is an function that indicates what "fraction" of the singularity is in the domain

Integration by Parts: RHS

- Recalling the approximation of the residual term, apply a similar procedure to the RHS:

$$\int_\Omega \hat{b} u_i^* = \sum_k \beta_k \int_\Omega \hat{f}_k u_i^* \quad (10)$$

$$= \sum_k \beta_k \int_\Omega -\Delta \hat{u}_k u_i^* \quad (11)$$

$$= \sum_k \beta_k \left[\int_\Gamma \hat{u}_k q_i^* - \hat{q}_k u_i^* + c(x_i) \hat{u}_k(x_i) \right] \quad (12)$$

Dual Reciprocity Integral Equation

Combining the LHS and RHS:

$$\int_\Gamma uq_i^* - qu_i^* + c(x_i)u(x_i) = \sum_k \beta_k \left[\int_\Gamma \hat{u}_k q_i^* - \hat{q}_k u_i^* + c(x_i)\hat{u}_k(x_i)\right] \quad (13)$$

- Using the method of collocation to distribute nodes on the boundary and cubic spline interpolation to interpolate between boundary nodes, the discretized equation becomes:

$$Hu + Gq = (H\hat{U} + G\hat{Q})\beta \quad (14)$$

Goals of Project

1. Integrate existing code used to solve the Stokes equation and Poisson equation:

$$-\nabla P + \mu \Delta \vec{v} + \rho \vec{b} = 0 \qquad \text{and} \qquad -\Delta u = b \tag{15}$$

   where b is harmonic

2. Use DRM to solve the Poisson equation for general $\hat{b} = b$
3. Use DRM to solve the heat equation

$$\frac{\partial}{\partial t} + \vec{v} \cdot \nabla u - \Delta u = b \qquad \text{where} \qquad \hat{b} = b - \frac{\partial}{\partial t} - \vec{v} \cdot \nabla u \tag{16}$$

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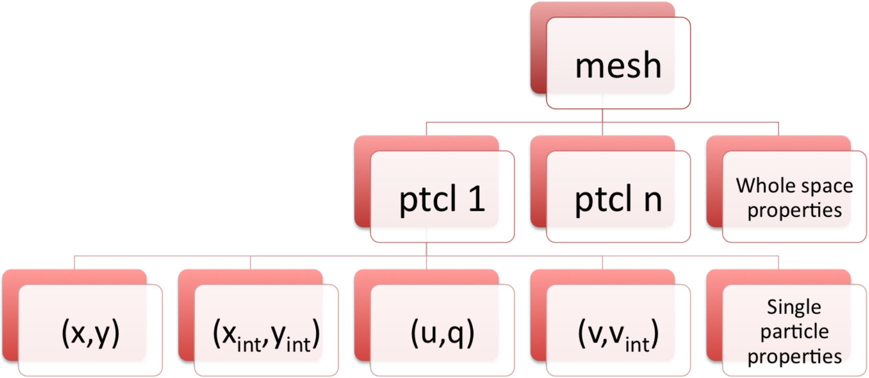
Goal 1: Integrate Solvers with Data Structures



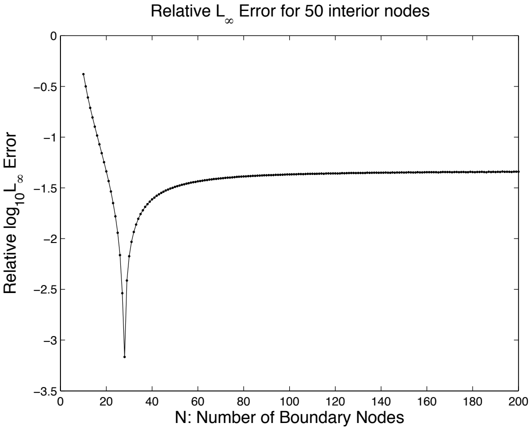
- Used to transfer information between solvers
- Very lean, contains only essential data
- Built to inspire code structure

Goal 1: Integrate Solvers with Subroutines

- Each code had different subroutines for the same task
  - Some functions appear hard coded multiple times
  - Required different inputs
  - Returned incompatible outputs
- Unified assembly routines
  - Matrices for the Stokes and heat equations are built in a similar manner
  - Learn one code, learn them both
- Replaced custom and Numerical Recipes methods with those found in LAPack and BLAS

Goal 2: Use DRM to Solve Poisson Equation

- Used to validate assembly of DRM matrices
- Spacial error was measured and analyzed



Goal 2: Use DRM to Solve Poisson Equation

- Noticed Error “bounce back"
  - Error decreases quadratically as number of nodes increased
  - Error then increases once a certain number of nodes is used
- Investigated potential causes
  - Recall $\beta = \hat{F}^{-1}b$
  - As N increases, $\kappa(\hat{F})$ increases leading to inaccurate β
- Solutions
  - Switch to double precision
  - Use different basis functions

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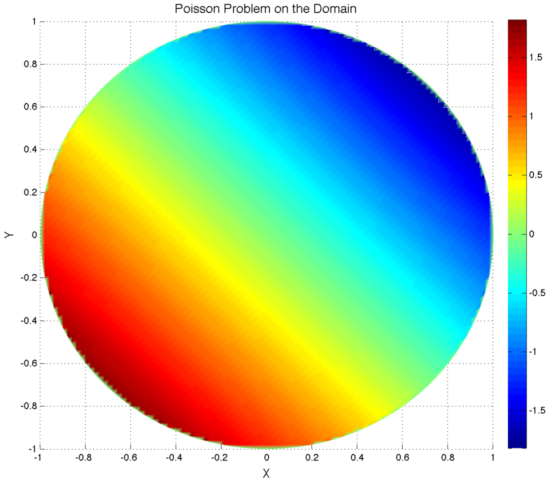

Goal 3: Use DRM to Solve Heat Equation

- Recall the DRM matrix equation

$$Hu + Gq = (H\hat{U} + G\hat{Q})\hat{F}^{-1}\hat{b} \tag{17}$$

where $\hat{b} = b - \frac{\partial}{\partial t}u - \vec{v} \cdot \nabla u$

- We want to discretize $\vec{v} \cdot \nabla u$
- Davis *et al.* showed the approximation

$$\frac{\partial}{\partial x}U = \frac{\partial \hat{F}}{\partial x}\hat{F}^{-1}U \quad \text{and} \quad \frac{\partial}{\partial y}U = \frac{\partial \hat{F}}{\partial y}\hat{F}^{-1}U \tag{18}$$

are valid

Goal 3: Use DRM to Solve Heat Equation

The DRM matrix equation for the heat equation becomes

$$Hu + Gq = (H\hat{U} + G\hat{Q})\hat{F}^{-1}\left(b - \frac{\partial}{\partial t}U - V_x \cdot \frac{\partial \hat{F}}{\partial x}\hat{F}^{-1}U - V_y \cdot \frac{\partial \hat{F}}{\partial y}\hat{F}^{-1}U\right) \quad (19)$$

- Notice that the linear system is a first order ordinary differential equation with variable t and unknown U
- Use Crank-Nicolson method to time step

Goal 3: Use DRM to Solve Heat Equation

- Used to validate time stepping method
- Time stepping error was measured and analyzed

Error Plot coming soon

Goal 3: Use DRM to Solve Heat Equation

Single particle movie: Still trying to figure out the technicalities of getting this in the slides

Goal 3: Use DRM to Solve Heat Equation

Multiparticle movie

Implementation Details

- Rewrote code to handle singular integrals
  - Generalized for use in Stokes and heat solvers
  - Optimized and debugged
- Implemented OpenMP
  - Matrix Assembly explicitly parallelized
  - Used the Intel Math Kernel Library for LAPack and BLAS which is parallelized with `-openmp` compile time flag
- Wrote domain back solver
  - Once boundary values are computed, domain values can be quickly back calculated
  - Separate program that shares many of the same libraries
- Provided detailed comments on code using Doxygen

Future Work

- Stokes solver currently not running
  - Separate modifications being one on the solver
  - Waiting until all modification to be complete before adding it solver
- No Fast Multipole Method
  - Makes the DRM linear systems sparse
  - Greatly increases code performance if systems are large
  - Current matrices from two dimensional problems are small
- Basis functions
  - Investigate using other basis functions
  - Functions with compact support
  - For whole space problems, basis functions should match asymptotically match the solution

Schedule

- Phase I (present - early November)
  - Merge Stokes flow and Poisson solver code ✔
- Phase II (November - December)
  - Test and validate steady-state code ✔
  - Optimize code ✔
- Phase III (December - early February)
  - Add Dual Reciprocity code ✔
  - Add Fast Multipole Method code (optional)
- Phase IV (February - March)
  - Test and validate Dual Reciprocity code ✔
  - Optimize code
    - Interface with Intel Math Kernel Library ✔
    - Parallel implementation with OpenMP ✔

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Questions?

Multiparticle movie here