Dual Reciprocity Boundary Element Method for Magma Ocean Simulations

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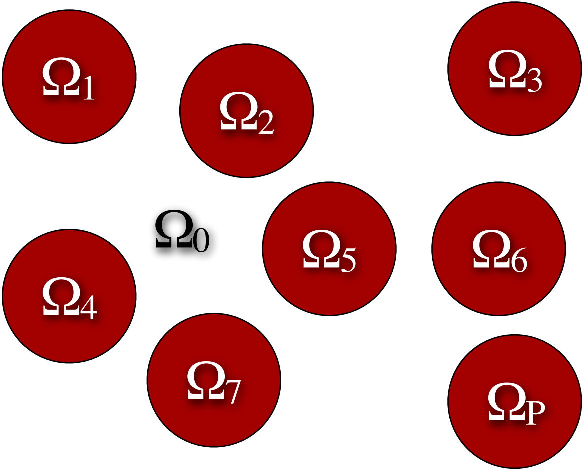
Overview

- Problem Description
  - Problem Geometry
  - Governing Equation
- Dual Reciprocity Boundary Element Method
  - Introduction for one domain
  - Matching domains
- Radial Basis Functions
  - Summary of the RBFs
- Numerical Methods
  - Discretization of Geometry
  - Numerical Integration
- Numerical Results
- Conclusion

Physical Motivation

- Giant impact between early Earth and Mars sized object
- Generated massive amounts of heat, formed global "magma ocean"
- Magma Ocean cooled partially by heat advection
  - Cooling first occurred at outer interface of magma ocean
  - Created dense, cold, crystals that settled into the ocean
  - Crystals may have been able to effective cool magma ocean at great depths
- Estimates on rate of cooling is not tight
  - Provide more accurate insight into Earth's early history
  - Present rates of cooling of the planet

Problem Geometry



Governing Equation

$$\frac{\partial u}{\partial t} + \boldsymbol{v} \cdot \nabla u - \kappa^p \nabla^2 u = b \quad \boldsymbol{x} \in \Omega^p \qquad p = \{0, 1, \ldots, P\} \qquad (1)$$

- Equation hold true for each crystal $p = (1, \ldots, P)$ and the suspension fluid $p = 0$.
- Each domain has constant heat conductivity κ
- BEM techniques exist for solving Stokes flow with multiple viscous particles in an infinite suspension
- New derived method based on Dual Reciprocity Boundary Element Method (DRBEM) for solving heat equation in similar domain

Boundary Conditions

- Between particle and suspension fluid
  - Potential is continuous across boundary
  - Flux is continuous across boundary
  - Boundary conditions are enforced in the linear system
- The suspension fluid at infinity
  - Regularity of solution required for unbounded DRBEM problems
  - Require solution to decay to zero sufficiently fast at infinity
  - Boundary condition enforced by removing boundary integral at infinity

Dual Reciprocity Boundary Element Method

- Approximates residual term by linear combination of Radial Basis Function (RBFs) such that

$$\sum_{j=1}^{N+L} \beta_j^p f_j^p \approx \hat{b} = b - \frac{\partial u}{\partial t} - \boldsymbol{v} \cdot \nabla u \qquad \text{and} \qquad \nabla^2 \hat{u}_j^p = f_j^p \quad (2)$$

- The new approximated heat equation can now be written

$$-\kappa^p \nabla^2 u = \sum_{j=1}^{N+L} \beta_j^p \nabla^2 \hat{u}_j^p \qquad p = \{0, 1, \ldots, P\} \qquad (3)$$

- BEM is applied to LHS as usual as well as to the RHS

Boundary Integral Equations

$$c_i^p u_j + \int_{\Gamma_p} \left[\left(\nabla u_j \cdot \hat{\boldsymbol{n}} \right) u_i^* - \left(\nabla u_i^* \cdot \hat{\boldsymbol{n}} \right) u_j \right] \mathrm{d}\Gamma_p =$$

$$\frac{1}{\kappa_p} \sum_{j=1}^{N_p+L_p} \beta_j^p \left(c_i^p \hat{u}_j^p + \int_{\Gamma_p} \left[\left(\nabla \hat{u}_j^p \cdot \hat{\boldsymbol{n}} \right) u_i^* - \left(\nabla u_i^* \cdot \hat{\boldsymbol{n}} \right) \hat{u}_j^p \right] \mathrm{d}\Gamma_p \right) \quad (4)$$

- The boundary integral equation holds for each domain of the problem
- The integral equation can be written as a linear system

$$H^p u^p - G^p q^p = (H^p \hat{U}^p - G^p \hat{Q}^p)\beta^p \quad (5)$$

Expanding the Coefficient Term

- Recall that

$$\beta^p = (F^p)^{-1}\hat{b} = (F^p)^{-1}\left(-\frac{\partial}{\partial t}u^p - V_x^p\nabla u^p - V_x^p\nabla u^p + b^p\right) \quad (6)$$

- V_x^p and V_y^p are diagonal matrices containing the velocities computed from the Stokes flow equation
- The gradient of the solution can be approximated using

$$\frac{\partial}{\partial x}U \approx \frac{\partial F^p}{\partial x}(F^p)^{-1} \qquad \frac{\partial}{\partial y}U \approx \frac{\partial F^p}{\partial y}(F^p)^{-1} \quad (7)$$

Interaction Between Domains

$$H^p u^p - G^p q^p = (H^p \hat{U}^p - G^p \hat{Q}^p)\beta^p \tag{8}$$

- The RHS of the linear equation is now equivalent to the domain integral of a source term of a Poisson equation that closely approximates the original residual term
- Require residual approximation to have desired properties
  - Source term is continuous between domains
  - Potential associated with source term is continuous across domains
  - Flux associated with source term is continuous across domains

Interaction Between Domains

- The residual term is matches at the boundary nodes due to collocation
- No guarantee that potential or flux match at boundary nodes
  - Add additional $3N_p$ harmonic functions to the potential approximation inside each particle
  - Use extra degrees of freedom to match potential and flux at boundary nodes
  - Harmonic functions do not alter original residual approximation
- Harmonic function ψ_j^p satisfy

$$\sum_{j=1}^{N_0+L_0} \beta_j^0 \hat{u}_j^0(x_i) = \sum_{j=1}^{N_p+L_p} \beta_j^p \hat{u}_j^p(x_i) + \sum_{j=1}^{3N_p} c_j^p \psi_j^p(x_i) \quad (9)$$

$$\sum^{N_0+L_0} \beta_j^0 \hat{q}_j^0(x_i) = \sum^{N_p+L_p} \beta_j^p \hat{q}_j^p(x_i) + \sum^{3N_p} c_j^p \nabla\psi_j^p(x_i) \cdot \boldsymbol{n}(x_i) \quad (10)$$

Matching Particle and Suspension

$$\begin{bmatrix} H_{\Gamma_p} & 0 \\ H_{\Omega_p} & I \end{bmatrix} \begin{bmatrix} u_{\Gamma_p} \\ u_{\Omega_p} \end{bmatrix} - \begin{bmatrix} G_{\Gamma_p} \\ G_{\Omega_p} \end{bmatrix} \begin{bmatrix} q_{\Gamma_p} \end{bmatrix} =$$

$$\left(\begin{bmatrix} H_{\Gamma_p} & 0 \\ H_{\Omega_p} & I \end{bmatrix} \begin{bmatrix} \hat{U}_{\Gamma_p\Gamma_p} & \hat{U}_{\Gamma_p\Omega_p} \\ \hat{U}_{\Omega_p\Gamma_p} & \hat{U}_{\Omega_p\Omega_p} \end{bmatrix} - \begin{bmatrix} G_{\Gamma_p} \\ G_{\Omega_p} \end{bmatrix} \begin{bmatrix} \hat{Q}_{\Gamma_p\Gamma_p} & \hat{Q}_{\Gamma_p\Omega_p} \end{bmatrix} \right) \begin{bmatrix} \beta_{\Gamma_p} \\ \beta_{\Omega_p} \end{bmatrix}$$

- Potential and flux is continuous across the boundary
- Each DRBEM linear system yields two equations
  - Solve first for the flux
  - Plug into second to relate boundary potentials to interior potentials
  - Match fluxes across boundary to match boundary nodes from the particles with those on the suspension

Radial Basis Functions (RBFs)

- Augmented Thin Plate Splines RBFs are used inside particles

$$f_j = r_j^2 \ln r_j \qquad \hat{\theta}_j = \frac{r^4 \ln r}{16} - \frac{r^4}{32} \tag{11}$$

  - Continuously differentiable
  - Augmented polynomial guarantees existence of solution
  - Numerically stable and robust

- Loeffler-Mansur RBFs are used in the suspension

$$f_j = \frac{2c - r_j}{(r_j + c)^4} \qquad \hat{\theta}_j = \frac{c + 2r_j}{2(r_j + c)^2} \tag{12}$$

  - Decay sufficiently to meet regularity requirements at infinity
  - Not differential at $r = 0$ (bounded but undefined)
  - Depends on parameter c that must be prescribed *a priori*

Interpolation

- Boundary is interpolated using cubic splines
  - Can be done individually for each particle in $\mathcal{O}(N)$ time
  - Approximated boundary is $\mathcal{C}^2$ allows for unit normal defined everywhere
- Non-fundamental solution functions approximated in integrals by linear Lagrange interpolation
  - More accurate than constant value approximation
  - Requires extra integration, but no work for computing interpolation functions
  - Allows for separation of fundamental solution integrals and functions in linear system formulation

Standard Integration

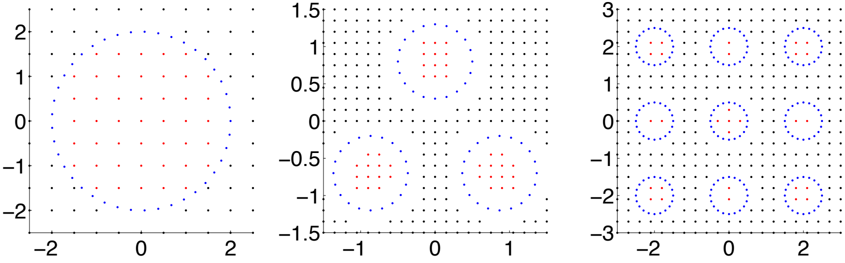
- Gaussian Quadrature
  - Handles standard, finite integrals with finite integrands
  - Eight point quadrature for high accuracy
  - Boundary element is interpolated at local quadrature points
  - Function is evaluated at global quadrature nodes
  - Allows for high precision

Singular Integration

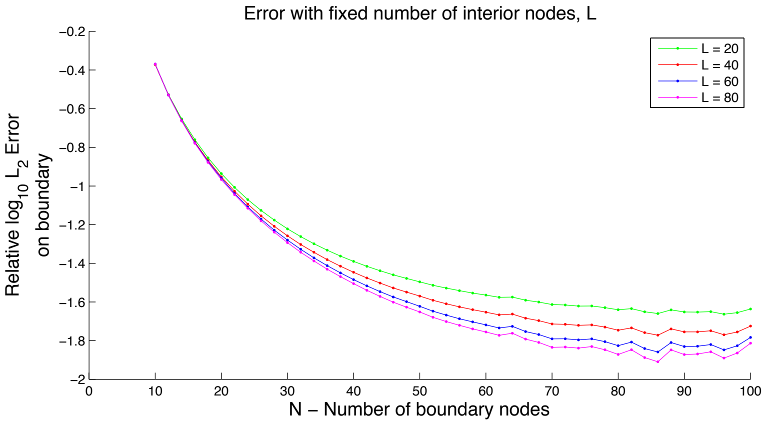
- Weakly singular integrals
  - Finite integrals with unbounded integrands
  - Ex: $\ln(r)$ in $\mathbb{R}^2$ problems and $1/r$ in $\mathbb{R}^3$
- Strongly singular integrals
  - Unbounded integrals with unbounded integrands
  - Finite in the Cauchy Principal Value sense
  - Ex: $1/r$ in $\mathbb{R}^2$ and $1/r^2$ in $\mathbb{R}^3$
- Evaluation using Radial Integration Method (RIM2D)
  - Finite part of integrand expanded as power series in r, the distance from the singularity
  - Singular part of integrand and integration variable transformed in terms of r
  - Results in evaluation of finite expressions

Problem Outline

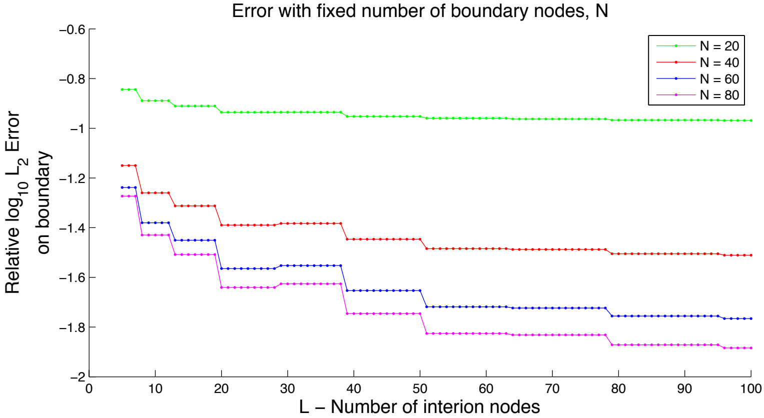
- Simulate cooling of one and three particles
- All problems start with temperature $\theta = 0$ in the suspension and $\theta = 1$ in the particles
- Time steps are sufficiently small to satisfy the CFL stability conditions



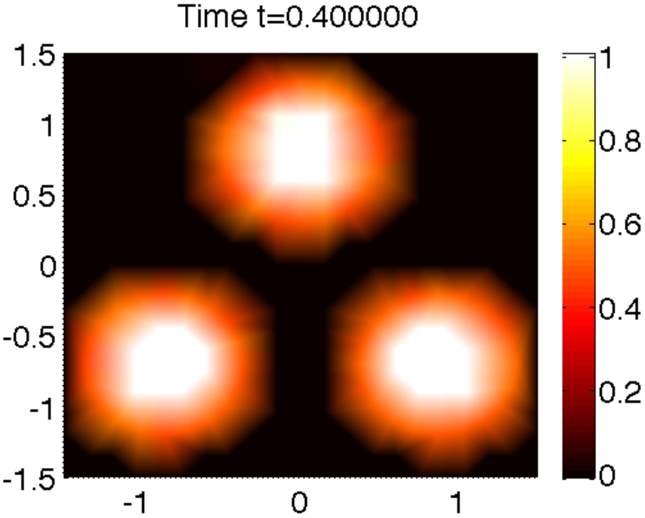
Validation For One Particle



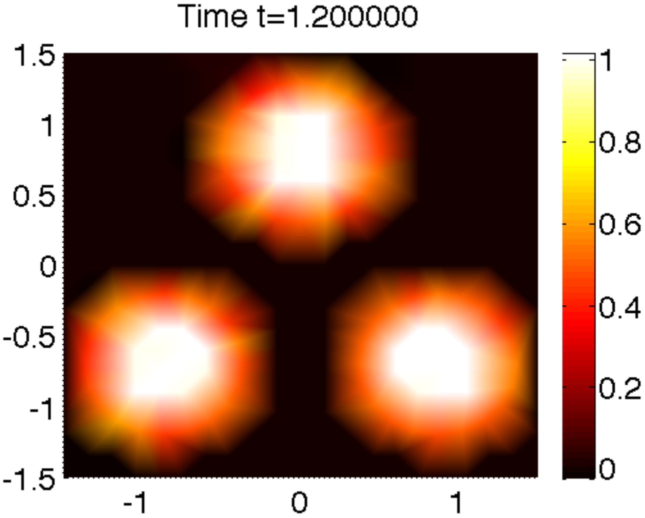
Validation For One Particle



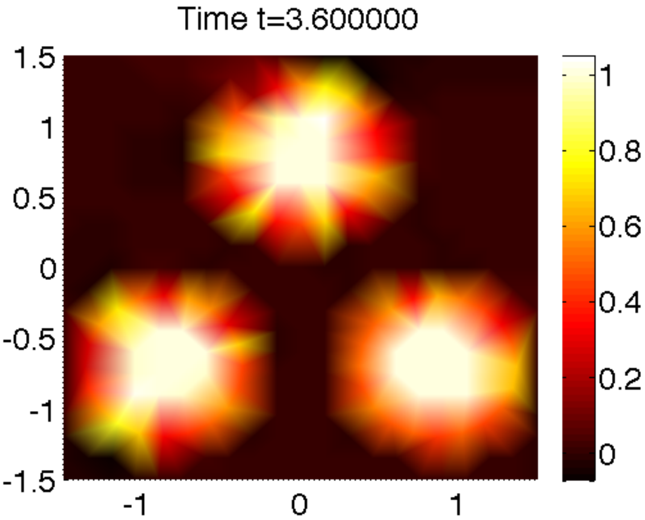
Results for Three Particles



Results for Three Particles



Results for Three Particles



Challenges

- Currently implemented as direct method
  - Must invert a matrix directly $\rightarrow \mathcal{O}(\mathcal{N}^4)$
  - Investigating sparse RBFs and fast methods (ACA,FMM)
- Domain RBFs contain parameter c
  - Too low and the method does not converge
  - Too high and the method becomes unstable
- LM RBFs cover "finite" amount of suspension
  - Decay very rapidly
  - Only approximate near computational nodes

Final Remarks

- New variation of the Dual Reciprocity Boundary Element Method will allow for accurate simulation of viscous particles settling into a suspension fluid
- Will be used to help find restraints on parameters needed to find answers about the early history of the planet
- Method can be applied to many other application areas that involve two phase fluid flow in infinite domains

Thank You

Questions?

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