Dual Reciprocity Boundary Element Method for Magma Ocean Simulations

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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
- It is being proposed to use the Dual Reciprocity Method as the basis for a numerical solver to address this problem.

Physical Motivation

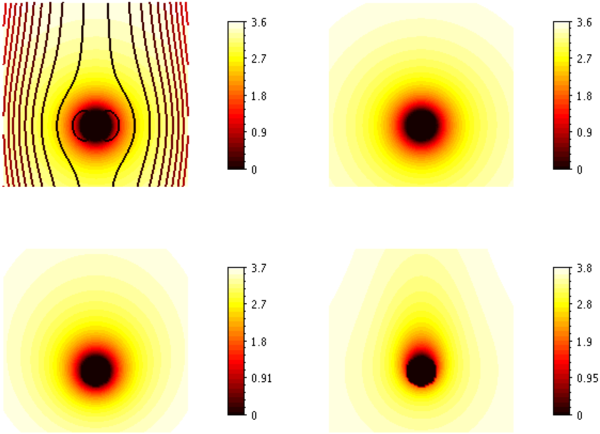
- Earth's early history is marked by a giant impact with a Mars-sized object
- This led to a substantial amount of interior melting followed by rapid crystallization of this 'magma ocean'
- How this crystallization took place and crystals settled provide insight into the planet's rate of cooling

Giant Impact

How to Solve

- Must solve a coupled Stokes flow and heat equation
- Settling crystals create a free boundary condition which makes traditional methods, such as FEM, a challenge to use
- First order accurate asymptotic solutions exists for limited parameters

Asymptotic Solution



Algorithm

- Boundary Element Method almost works
  - Naturally handles free boundaries
  - Approximation performed on only on the boundary
  - Cannot handle transient heat equation with source term
- Dual Reciprocity Method fits the problem
  - Naturally handles free boundaries
  - Approximation performed on only on the boundary
  - Can solve transient heat equation with source term

The Set Up

Given a non-linear PDE

$$\mathcal{D}u = b \tag{1}$$

Rewrite it as a combination of a linear operator $\mathcal{L}$ and non-linear residual operator $\mathcal{D}'$

$$\mathcal{L}u = b - \mathcal{D}'u =: b' \tag{2}$$

Define b', the combination of original source with the non-linear operator, to be the new source term to the linear PDE

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The Heat Equation

Consider the heat equation

$$\frac{\partial}{\partial t}u + \vec{v} \cdot \nabla u - \Delta u = b \tag{3}$$

Break it down into a linear operator and its residual

$$\mathcal{D} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla - \Delta \tag{4}$$

$$\mathcal{L} = -\Delta \tag{5}$$

$$\mathcal{D}' = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \tag{6}$$

$$b' = b - \frac{\partial}{\partial t}u - \vec{v} \cdot \nabla u \tag{7}$$

Formulating Integral Equations

Form the Boundary Integral Equation using the linear PDE

$$-\Delta u = b' \qquad x \in \Omega \tag{8}$$

$$-\Delta u \cdot w = b' \cdot w \tag{9}$$

$$-\int_\Omega \Delta u \cdot w \, \mathrm{d}\Omega = \int_\Omega b' \cdot w \, \mathrm{d}\Omega \tag{10}$$

Perform integration by parts twice on the left hand side

$$\begin{aligned} \int_\Omega \Delta u \cdot w \, \mathrm{d}\Omega &= \int_\Gamma w D u \cdot \vec{n} \, \mathrm{d}\Gamma - \int_\Omega D u \cdot D w \, \mathrm{d}\Omega \\ &= \int_\Gamma (w D u - u D w) \cdot \vec{n} \, \mathrm{d}\Gamma + \int_\Omega u \Delta w \, \mathrm{d}\Omega \end{aligned}$$

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Perform integration by parts twice on the left hand side

$$\begin{aligned} \int_\Omega \Delta u \cdot w \, \mathrm{d}\Omega &= \int_\Gamma w D u \cdot \vec{n} \, \mathrm{d}\Gamma - \int_\Omega Du \cdot Dw \, \mathrm{d}\Omega \\ &= \int_\Gamma (wDu - uDw) \cdot \vec{n} \, \mathrm{d}\Gamma + \int_\Omega u \Delta w \, \mathrm{d}\Omega \end{aligned}$$

Fundamental Solutions

Choose $w = u^*$ where u^* is the fundamental solution to the adjoint operator $\mathcal{L}^*$

$$\Delta u^* = -\delta(x - \xi) \tag{11}$$

then

$$u(\xi) = \int_\Gamma (u^* Du - u Du^*) \cdot \vec{n} \, d\Gamma + \int_\Omega b' u^* \, d\Omega \tag{12}$$

for $\xi \in \Omega$

Approximation of Source

- Converted the linear term to the boundary
- Still need to convert source term to boundary
  - Given particular solution to $\mathcal{L}u' = b'$ is know this is possible
  - Particular solution is almost never known
- Dual Reciprocity approximates the source term by a linear combination of functions for which a particular solution is known

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Properties of Approximation

Approximate the source term b'

$$b' = \sum_{q=1}^{\mathcal{N}} f^q \alpha_q \tag{13}$$

Choose basis function f^q such that the particular solution u^q is known

$$\Delta u^q = f^q, \tag{14}$$

Then the original PDE becomes

$$-\Delta u = \sum_{q=1}^{\mathcal{N}} f^q \alpha_q \tag{15}$$

Substitution

Substituting for b' the integral equation becomes

$$u(\xi) = \int_\Gamma (u^* Du - uDu^*) \cdot \vec{n} \, \mathrm{d}\Gamma + \sum_{q=1}^{\mathcal{N}} \alpha_q \int_\Omega f^q u^* \mathrm{d}\Omega \qquad (16)$$

Substituting for f^p

$$u(\xi) = \int_\Gamma (u^* Du - uDu^*) \cdot \vec{n} \, \mathrm{d}\Gamma - \sum_{q=1}^{\mathcal{N}} \alpha_q \int_\Omega \Delta u^q u^* \mathrm{d}\Omega \qquad (17)$$

The Second Reciprocity Equation

Using the second Gauβ theorem

$$\int_\Omega (\Delta u^q u^* - \Delta u^* u^q)\ \mathrm{d}\Omega = \int_\Gamma (Du^q u^* - Du^* u^q) \cdot \vec{n}\ \mathrm{d}\Gamma \tag{18}$$

Which, after remembering the choice of u^*, becomes

$$\int_\Omega \Delta u^q u^*\ \mathrm{d}\Omega = -u^q(\xi) + \int_\Gamma (Du^q u^* - Du^* u^q) \cdot \vec{n}\ \mathrm{d}\Gamma \tag{19}$$

Substituting into the integral equation yields...

Dual Reciprocity

The Dual Reciprocity equation

$$\begin{aligned} u(\xi) &= \int_\Gamma (u^* Du - uDu^*) \cdot \vec{n} \, \mathrm{d}\Gamma \\ &\quad + \sum_{q=1}^{\mathcal{N}} \left(u^q(\xi) - \int_\Gamma (Du^q u^* - Du^* u^q) \cdot \vec{n} \, \mathrm{d}\Gamma \right) \alpha^q \end{aligned}$$

for $\xi \in \Omega$

Computation

- Equations are non-dimensionalized
- Discretized using the method of collocation ($\xi \rightarrow \Gamma$)
- Yields a linear system of N equations and N unknowns where N is the number of discretized elements
- All known and unknown values are on the boundary
- BEM formulation provides a method for approximating values in the region once unknown values are found

Challenges

- Linear systems involve dense and asymmetric matrices
  - *LU*-Decomposition with pivoting for stable backward and forward substitution
  - Fast Multipole Method demands extra upfront work but generates a sparse linear system (optional)
- Weakly and Strongly singular integrals
  - Appear from collocation ($\xi \rightarrow \Gamma$)
  - Iterative methods
  - Radial approximation techniques

Runtime

- Dominated by calculation of matrix and solving the associated linear system
  - $\mathcal{O}(N^2)$ with dense matrices
  - $\mathcal{O}(N \log N)$ with FMM
    - $\mathcal{O}(N)$ - upfront work
    - $\mathcal{O}(N \log N)$ - compute entries of sparse matrix
    - $\mathcal{O}(N)$ - solve using sparse solver such as GMRES

Platform

- Software: Fortran 90
  - Very fast execution
  - Object Orientated
  - Existing BEM Poisson and Stokes flow solver
- Hardware: Single core x86 architecture
  - Readily available
  - Local access to 32 node x86 cluster
  - Scalable from netbooks to supercomputers

Test Data

- Use initial conditions and parameters from literature
  - Modify these conditions and parameters as experimentation demands
- Parameters for asymptotic approximations for steady-state Stokes flow and heat problems

Validation

- Test steady-state code
  - Validate new Poisson and Stokes portion
    - Test Poisson code in isoviscous environment
    - Test Stokes code in isothermal environment
  - Use asymptotic approximations for non-isoviscous and non-isothermal problem

Validation

- Test Dual Reciprocity code
  - Use test functions
    - Create test function v
    - Compute $v_0 = v(t = 0)$ and $\mathcal{D}v =: b$
    - Then v is an exact solution to $\mathcal{D}u = b$ with $u(t = 0) = v_0$

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

Deliverables

- Collection of source and compiled libraries
  - Validated and optimized
  - Easily modifiable and modular
  - Robust and reusable
  - Platform for further research and development
- Reports
  - AMSC664 Report
  - Geophysics paper detailing methods and results for physical simulations
- Presentations
  - AMSC664 Presentation
  - Presenting paper at 12^{th} International Workshop on Modeling of Mantle Convection and Lithospheric Dynamics in Berlin, Germany, Summer 2011

D. Nardini and C. A. Brebbia, “A new approach to free vibration analysis using boundary elements", *Boundary Element Methods in Engineering*, Volume 7, Issue 3, 1983, Pages157-162

D. Nardini and C. A. Brebbia, “Transient dynamic analysis by the boundary element method", *Boundary Elements*, 1983, Pages 719-730

D. Nardini and C. A. Brebbia, “Boundary integral formulation of mass matrices for dunamic analysis", *Topics in Boundary Element Research*, Volume 2: Time-Dependent and Vibration Problems, 1985, Pages 191-208

D. Martin and R. Nokes. “A Fluid-Dynamical Study of Crystal Settling in Convecting Magmas", *Journal of Petrology*, Volume 30, Issue 6, 1989, Pages 1471-1500

C. Pozrikidis, *Boundary integral and singularity methods for linearized viscous flow*, Cambridge University Text, New York, NY, 1992

G. Leal, *Laminar Flow and Convective Transport Processes*, Butterworth-Heinemann, 1992

M. Manga and H. A. Stone, “Buoyancy-driven interactions between two deformable viscous drops", *Journal of Fluid Mechanics*, Volume 256, 1993, Pages 647-683

V. Solomatov and D. Stevenson, “Suspension in Convective Layers and Style of Differentiation of a Terrestrial Magma Ocean", *Journal of Geophysical Research*, Volume 98, Issue E3, 1993, Pages 5375-5390

V. Solomatov and D. Stevenson, “Nonfractional Crystallization of a Terrestrial Magma Ocean", *Journal of Geophysical Research*, Volume 98, Issue E3, 1993, Pages 5391-5406

V. Solomatov and D. Stevenson, “Kinetics of Crystal Growth in Terrestrial Magma Ocean", *Journal of Geophysical Research*, Volume 98, Issue E3, 1993, Pages 5407-5418

J. P. Agnantiaris, D. Polyzos, D. E. Beskos, “Three-dimensional structural vibration analysis by the Bual Reciprocity BEM", *Computational Mechanics*, Volume 21, Issue 4-5, 1998, Pages 372-381

M. A. Golberg, C. S. Chen, H. Bowman and H. Power, “Some comments on the use of Radial Basis Functions in the Dual Reciprocity Method", *Computational Mechanics*, Volume 21, Issue 2, 1998, Pages 141-148

R. M. Canup and E. Asphaug, “Origin of the Moon in a giant impact near the end of the Earths formation", *Nature*, Volume 412, 2001, Pages 708-712

L. T. Elkins-Tanton, E. M. Parmentier, and P. C. Hess, “Magma ocean fractional crystallization and cumulate overturn in terrestrial planets: Implications for Mars", *Meteoritics & Planetary Science*, Volume 38, Issue 12, 2003, Pages 1753-1771

L. Gaul, M. Kögl, M. Wagner, *Boundary Element Methods for Engineers and Scientists*, Springer, Berlin, 2003

Y. J. Liu and N. Nishimura, “The fast multipole boundary element method for potential problems: A tutorial", *Engineering Analysis with Boundary Elements*, Volume 30, Issue 5, May 2006, Pages 371-381

Xiao-Wei Gao, “Numerical evaluation of two-dimensional singular boundary integrals-Theory and Fortran code", *Journal of Computational and Applied Mathematics*, Volume 188, Issue 1, 2006, Pages 44-64

V. Solomatov, “ Magma Oceans and Primordial Mantle Differentiation", *Treatise on Geophysics*, Volume 9, 2007, Pages 91-120

Thank You

Questions?