Dual Reciprocity Boundary Element Method for Magma Ocean Simulations

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Abstract

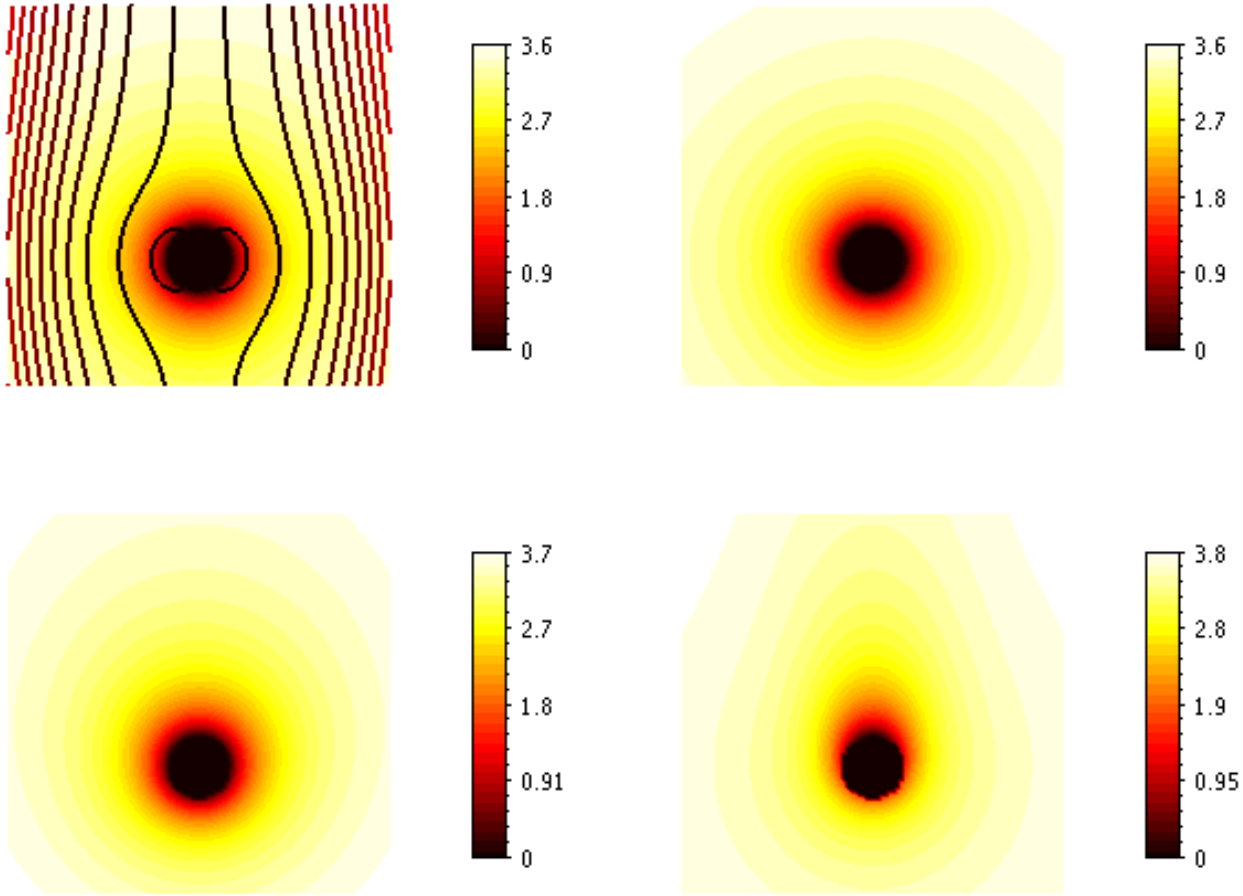
- Understanding how crystals settle in a magma ocean is critical for answering questions about Earth's early history
- Experiments have been performed that have given insight into this behavior
- The ability to simulate this behavior numerically is not available
- It has been proposed to use Dual Reciprocity Method as the basis for a numerical solver to address this problem.

Physical Motivation

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



Dual Reciprocity

Boundary Element Stokes equation

$$\vec{v}(\xi) = \int_{\Gamma} \Delta f \cdot \underline{J} \, \mathrm{d}\Gamma + \frac{1-\lambda}{1+\lambda} \int_{\Gamma} \vec{n} \cdot \mathbf{K} \cdot v \, \mathrm{d}\Gamma$$

The Dual Reciprocity equation

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

Where we started

- Two separate codes
  - BEM code for solving Poisson equation with harmonic source term
  - BEM code for solving Stokes' flow equation
- Incompatibilities
  - Different data structures
  - Different subroutines with same purpose
  - Stokes: Many particle; Poisson: One particle
- Inefficiencies
  - Recalculation of geometry information
  - High memory usage

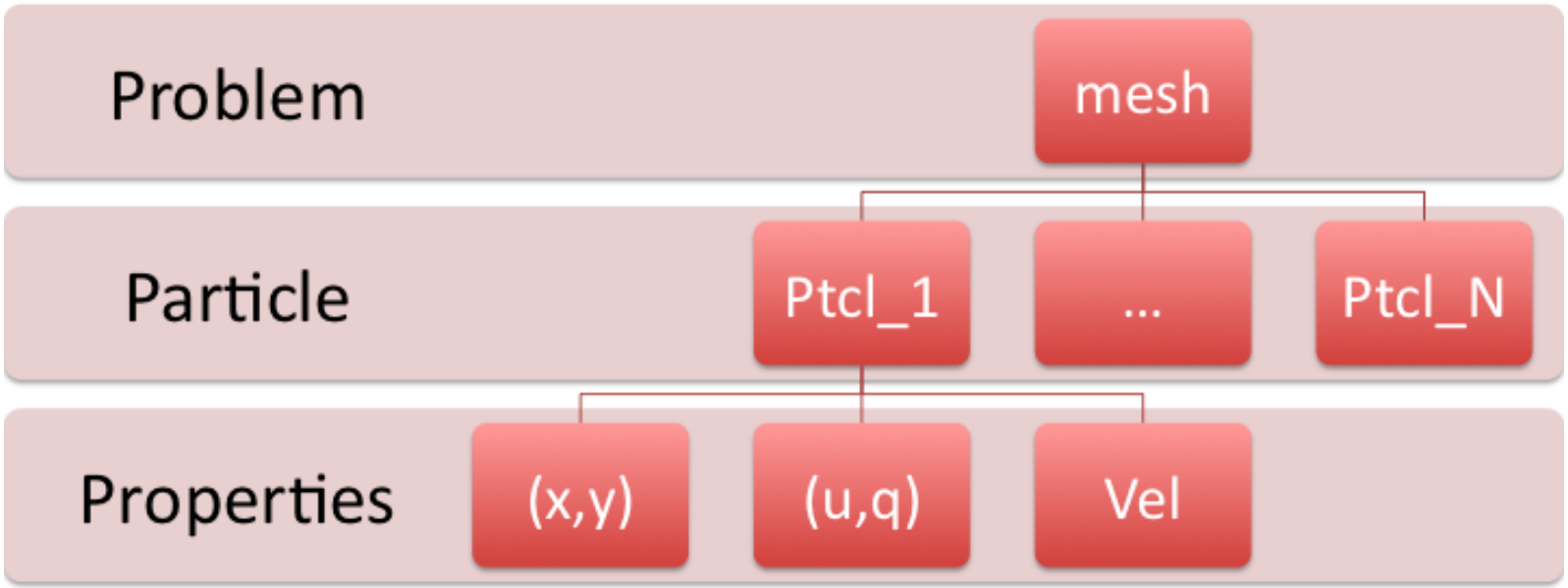
Work to do

- Stokes solver is generally better that Poisson
  - Robust
  - Efficient
  - Modular
- Rebuild Poisson to incorporate good traits
  - Advanced problem data structure
  - Unified subroutines
  - Remove large inefficiencies

Data Structures

- Wanted to take advantage of OO in Fortran 90
- One "problem" variable to share between the solvers
- Include all important information while being minimal
- Flexible to allow for large variety of simulations

Data Structures



- Each particle has independent parameters

Merging Subroutines

- Many subroutines for
  - Cubic spline interpolation
  - Tangent and normal vector computation
  - Gaussian integration
  - Radial integration (for singular integrals)
- Unified across two solvers
  - Minimal changes to routine interfaces
  - Overloading of routines in limited cases
  - Removed hard coded duplication of routines

An Example - Radial Integration Method

- Originally:
  - Stokes:
    `rim2d(xpole,ypole,xi,x,y,tx,ty,fx,fy,kern,plfrst)`
  - Poisson:
    `rim2d(xj,yj,xpole,ypole,d2x,sj,spole,kj,kpole,I,n,b,counter)`
- Currently:
  - Stokes:
    `rim2d(xa,ya,fx,x2a,y2a,arca,xb,yb,fy,x2b,y2b,arcb,plfirst,kern)`
  - Poisson:
    `rim2d(xa,ya,x2a,y2a,arca,xb,yb,x2b,y2b,arcb,plfirst,kern)`
- Both functions behave exactly the same internally

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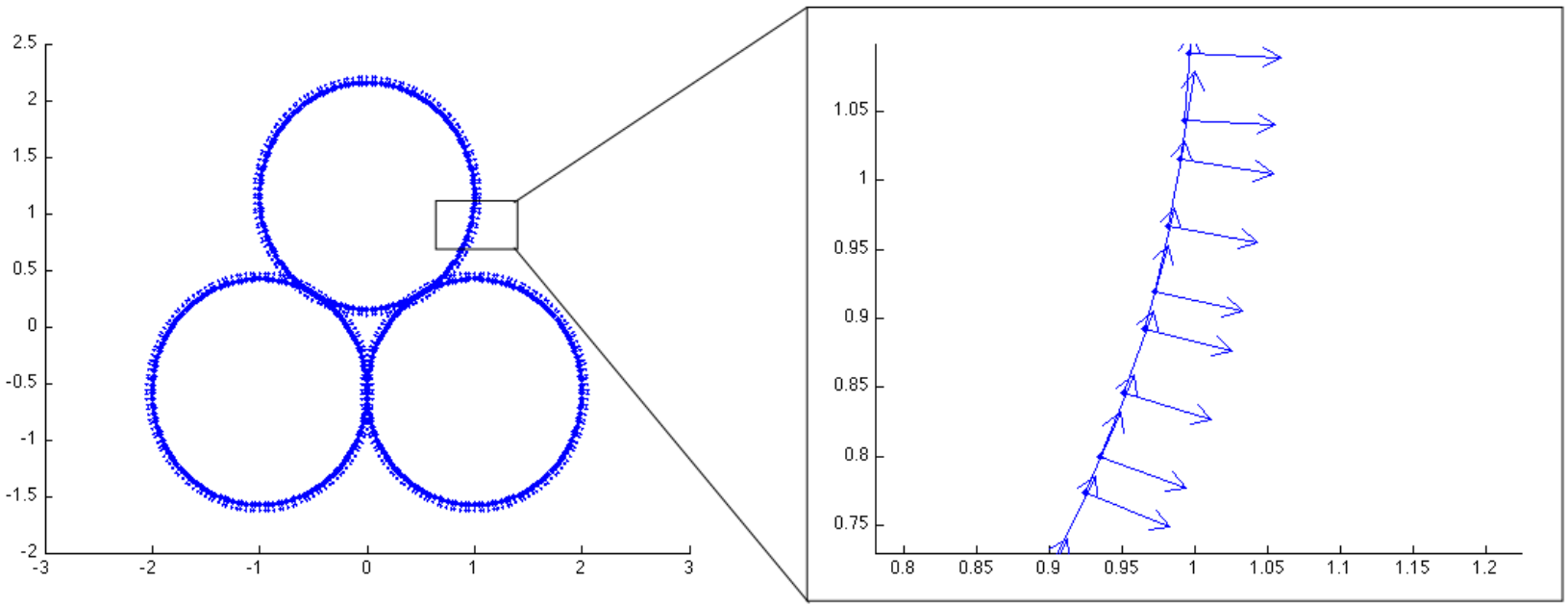
Expanded to many particles

- Data structure provided guidance for matrix assembly loop structure
- Required few high-level changes in matrix assembly code, no new subroutines required



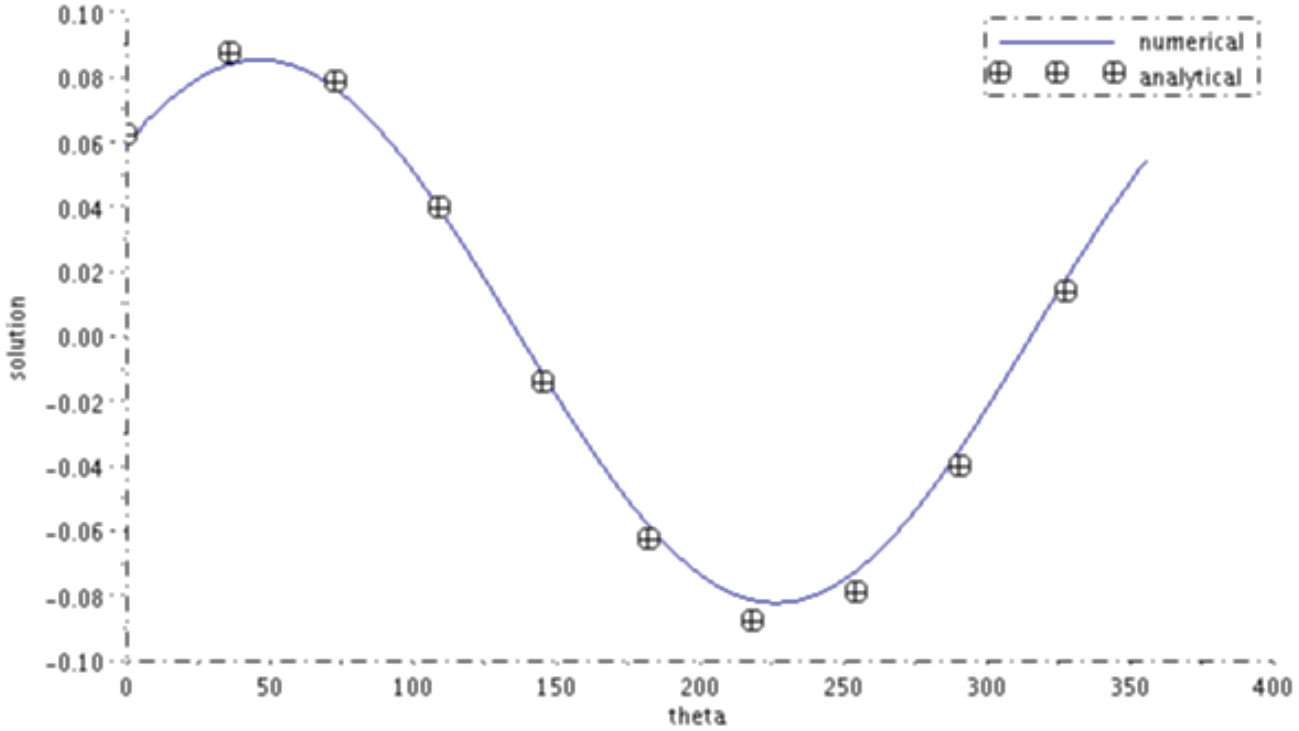
Inefficiencies in Poisson solver

- Inefficiencies for large problems
  - Recalculating geometry multiple times
  - Storing unused geometry data
  - Recomputing many basic values unnecessarily
- Fixed by switching orders of loops
  - No global geometry data computed or stored up front
  - Minimal particle geometry data computed once
  - Detailed geometry computed on the fly for small parts of the boundary
  - On the fly computation done exactly once
- Switches assembly routine from row based to column based

Validation

- Can validate against exact solution for specific Neumann boundary conditions and boundary shape
- Let Ω be the disk of radius 1 with
  - $b = a_1 x + a_2 y$
  - $q = -\frac{1}{8}(a_2 x + a_1 y)$
- Then the potential is given by
  - $u = \frac{1}{8}(a_1 x + a_2 y)$

Validation



$$a_1 = a_2 = 0.5$$

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
  - New code base is clean and compact
  - "Build up" from existing code slowly and carefully adding functionality without repeat code
- Scientific Results
  - Multiparticle Poisson solver


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?