

I have two main areas of research interest. One is the formulation of fast numerical algorithms for partial differential equations stemming from physical applications. The other is the construction of efficient numerical linear algebra algorithms applied to engineering problems. Papers, pre-prints, and other material indicated as available online can be found at:

<http://www-rocq.inria.fr/~jli/>

1 Numerical methods for PDEs

1.1 Acceleration of time/space convolutions for the heat equation

One of my principal areas of interest has been the solution of the heat equation, particularly in moving and/or unbounded domains. The challenge of problems posed on unbounded domains comes from the fact that using prevalent methods such as finite elements or finite difference methods, it can be difficult to couple the interior mesh to a high order discretization of transparent boundary conditions on an artificial boundary while maintaining stability. The challenge for discretizing moving boundaries is similar, namely the difficulty in obtaining high order and stable numerical schemes.

The approach of this research is the fast computation of the integral representation of the solution of the heat equation, which naturally takes into account the problem domain (possibly unbounded) and the boundary (possibly moving). For example, diffusion of heat into an infinite domain is automatically satisfied; there is no need for artificial boundary conditions. Similarly, a moving boundary means that one needs to compute integrals over this boundary and this can be done in a stable fashion.

This approach is suitable for the linear piece-wise constant coefficient heat equation, which occurs in numerous applications. The bottleneck of such an approach is the algorithmic complexity and memory requirements of computing time and spatial convolution integrals. This research focuses on accelerating both the time and spatial convolutions associated with the heat problem. The acceleration of the time convolution comes from computing the smooth part of the integral in the Fourier domain—coupling an efficient quadrature of the Fourier integral appropriate for unbounded domains with the Non-uniform FFT. We also developed an accurate quadrature for the non-smooth part of layer potential integrals—the goal being the treatment of domains whose geometrical properties may cause simpler time quadratures to suffer from slow convergence. The acceleration of spatial convolution is obtained by using the Fast Gauss Transform and other fast algorithms (still to be developed) treating the appropriate kernels.

The resulting algorithm has $O(MN \log N)$ complexity, where N is the number of spatial discretization points and M the number of time steps, a significant improvement over the $O(M^2 N^2)$ complexity of a naive implementation.

Collaborators: Leslie Greengard, Courant Institute of Mathematical Sciences. Code contains subprograms based on the Fast Gauss Transform (Greengard and John Strain, Univ. of California at Berkeley) and an implementation of the Non-uniform FFT (Greengard and June-Yub Lee, Ewha Womans University).

Publications

1. *Fast and accurate computation of layer heat potentials*, J.-R. Li, L. Greengard. Submitted. Preprint online.
2. *On the numerical solution of the heat equation I: fast solvers in free space*, L. Greengard, J.-R. Li, *Journal of Computational Physics*, Vol. 226-2, 1 Oct. 2007.

1.2 Application to the modeling of dendritic solidification

The modeling of dendritic solidification is a perfect application for the fast heat equation solver we developed. We will take as an example a particular model for this physical process, called the phase field model.

The phase field model consists of a coupled system of two heat equations: the one governing the thermal field is linear and constant coefficient, the one governing the phase variable is nonlinear. Current methods use finite differences or finite elements to treat both equations. Difficulty occurs when one wants to simulate the solidification when the liquid is cooled to just slightly below its melting temperature. In this 'low undercooling' case, the solidification is slow. The solid-liquid interface moves slowly whereas the thermal field expands rapidly. In the absence of correctly

formulated artificial boundary conditions, a finite differences/elements discretization of both equations is required to include in the computational domain the entire extent of the thermal field, which is much larger than the solidification front, the object of interest. For very low undercoolings, current methods based on finite differences/elements are not computational practical. A quote [from Braun and Murray, *Journal of Crystal Growth*, 1997] on adding adaptivity to simulate low undercoolings is illustrative of the potential difficulty: *Another issue that needs to be addressed in these types of simulations is the disparity between the dendrite size and the extent of the thermal field at small undercoolings. The larger domains and longer times allowed by adaptivity did not entirely solve this problem, and a more sophisticated mathematical approach for treating the domain boundary is required for computation at very small undercoolings.*

We believe our fast heat equation solver provides the sorely needed 'more sophisticated mathematical approach'. We have used the fast heat solver for the thermal field equation and coupled it to a finite difference method for the phase variable equation. In essence, the thermal field is allowed to correctly diffuse out of the computational domain, by construction. We then showed the feasibility of simulating the difficult case where the liquid experiences very low undercooling.

Collaborators: Lucien Brush, Dept. of Materials Science, University of Washington. Donna Calhoun, Commissariat à l'Énergie Atomique, Paris.

Publications

1. *Efficient thermal field computation in phase field models*, J.-R. Li, D. Calhoun, L. Brush. *Submitted. Preprint online.*

1.3 Fractional differential equations

We can extend the spectral representation developed for the heat kernel to other fractional power kernels and use the representation in the solution of general equations containing fractional integrals and derivatives (which appear, for example, in the modeling of viscoelastic materials). This involves constructing a Fourier quadrature for arbitrary fractional coefficients (whereas for the heat kernel, this coefficient is $\frac{1}{2}$). Additionally, the density in the convolution integral will be singular (in time) and must be treated appropriately. (For the heat equation, we had smooth densities). I have implemented this approach and will make numerical comparisons with existing methods which use other ways of accelerating the time convolution.

Publications

1. *A fast time stepping method for evaluating fractional integrals*, J.-R. Li. *Submitted. Preprint online.*
2. *Efficient solution of a wave equation with fractional order dissipative terms*, H. Haddar, J.-R. Li, D. Matignon. *Accepted by the Journal of Computational and Applied Mathematics. Preprint online.*

1.4 High order marching methods to solve the wave equation on embedded Cartesian grids

One of the most straightforward methods for solving partial differential equations in complex geometry is simply to superimpose the geometry on a Cartesian mesh, with a distinct representation of the surface ("embedded Cartesian grids"). It has been extremely difficult, however, to obtain methods for hyperbolic equations, including the scalar wave equation, that are stable, explicit and high-order accurate. The design of such methods has been a focus of my work.

Due to small cells near the boundary of the problem domain, if one uses a fixed stencil at all grid points, the resulting CFL condition is overly restrictive, since it is based on the size of the smallest spatial cell. Stability is also difficult to obtain. I analyzed and refined a class of explicit three-step schemes which rely on an integral evolution formula for which the numerical domain of dependence adjusts automatically to contain the true domain of dependence. In this way, the size of the allowable time step can be on the order of the size of the typical spatial cell in the uniform part of the Cartesian grid. I have implemented such schemes to high order (up to 6th order) for complex geometry in two

dimensions and found them to be numerically stable.

Collaborators: Leslie Greengard, Courant Institute of Mathematical Sciences.

Publications

1. *High order marching schemes for the wave equation in complex geometry*, J.-R. Li, L. Greengard, *Journal of Computational Physics*, Volume 198-1, 20 July 2004.
2. *Strongly consistent marching schemes for the wave equation*, J.-R. Li, L. Greengard, *Journal of Computational Physics*, Volume 188-1, 10 June 2003.

1.5 Exact boundary conditions for Helmholtz equation in local perturbed periodic media; related topic: the efficient implementation of transparent boundary conditions for the time-domain wave equation

Another research topic is finding artificial (but exact) boundary conditions for periodic waveguides with local perturbations. This is achieved by constructing Dirichlet-to-Neumann operators for the infinite waveguide outside the local perturbation—by solving (many) local problems (the Helmholtz equation) posed on a single periodicity cell.

The method has been implemented for two dimensional waveguides using rectangular mixed finite elements. The waveguides are periodic in one spatial direction, the extension the work to materials which are periodic in two spatial dimensions, such as photonic crystals, is the research topic of the Ph.D. student Sonia Fliss.

I have also worked on finding accurate low order rational approximations to the logarithmic derivative of Hankel functions, which are needed for the fast evaluation of the convolution integrals in certain transparent boundary conditions for the wave equation. In particular, I used the Balanced Truncation method from model reduction to generate low order approximations for the half-order Hankel functions, resulting in small errors and poles which are all (provably) stable.

Collaborators: Patrick Joly, Sonia Fliss, INRIA.

Publications

1. *Exact boundary conditions for periodic waveguides containing a local perturbation*, P. Joly, J.-R. Li, S. Fliss, *Commun. Comput. Phys.*, 1 2006.
2. *Low order approximation of the spherical nonreflecting boundary kernel for the wave equation*, J. Li, *Linear Algebra and its Applications*, Special Issue on Order Reduction of Large-Scale Systems, Volume 415, Issues 2-3, June 2006.

2 Numerical linear algebra

2.1 Low rank solution of Lyapunov equations

As part of my thesis work, I reformulated the classical ADI method for the solution of Lyapunov equations to specifically solve equations which have low rank right-hand sides, so that the new formulation, Cholesky-Factor ADI, requires only linear matrix-vector solves rather than the full matrix operations required by the classical method. I also showed that the Cholesky-Factor ADI algorithm can be implemented as the simultaneous solution of many shifted systems with the same right hand side, and showed that a single Krylov subspace can be used to iteratively solve all shifted systems via GMRES.

This work resulted in the article *Low rank solution of Lyapunov equations* which was chosen as a SIGEST selection in the SIAM Review in 2004. For this work I also received the Alston Householder Award for the best dissertation in Numerical Algebra (2002) and the Leslie Fox Prize in Numerical Analysis (Second Prize, 2001).

Collaborators: Jacob White, Dept of Elec. Engin., MIT.

Publications:

1. *Numerical solution of large-scale Lyapunov equations, Riccati equations, and linear-quadratic optimal control problems*, P. Benner, J.-R. Li, T. Penzl, *Numerical Linear Algebra with Applications*, Volume 15, 2008, Pages 755-777.
2. *Low rank solution of Lyapunov equations*, J.-R. Li, J. White, *SIAM Review*, SIGEST selection, issue 46-4, December 2004.
3. *Low rank solution of Lyapunov equations*, J.-R. Li, J. White, *SIAM Journal on Matrix Analysis and Applications*, **24** 2002.

2.2 Application to problem of model reduction of large circuit systems

I proposed a new method for the model reduction of large circuit systems called the Dominant Gramian Eigenspaces method, which utilizes low rank approximations to the exact system Gramians. The Cholesky Factor ADI algorithm was used to generate low rank approximations to the system Gramians. I showed that in a model reduction method for symmetric systems based on moment matching, the problem of choosing moment matching points can be approached by solving the rational min-max problem associated with CF-ADI parameter selection.

The reduction of model size is essential to the design and simulation of these systems.

Collaborators: Jacob White, Dept of Elec. Engin., MIT.

Publications:

1. *Smith-Type methods for balanced truncation of large sparse systems*, S. Gugercin, J.-R. Li, *Dimension Reduction of Large-Scale Systems Proceedings of a Workshop held in Oberwolfach, Germany, October 19-25, 2003*.
2. *Reduction of large circuit models via low rank approximate Gramians*, J.-R. Li, J. White, *International Journal of Applied Math. and Comp. Sci.*, **11**, 2001.
3. *Efficient Model Reduction of Interconnect via Approximate System Grammians*, J.-R. Li, J. White, *IEEE/ACM International Conference on Computer-Aided Design, 1999. Digest of Technical Papers. 7-11 Nov. 1999*.
4. *An Efficient Lyapunov Equation-Based Approach for Generating Reduced Order Models of Interconnect*, J.-R. Li, F. Wang, J. White, *Design Automation Conference, 1999. Proceedings. 36th, 21-25 June 1999*.