"Scalable multi-resolution solvers for inverse problems for Systems governed by reaction-diffusion equations: Applications to inverse problems in electrophysiology"

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Summary

Inverse problems constrained by reaction-diffusion equations have numerous applications in science and engineering. Although there is a rich body of work on numerical methods for the forward problem, there exists limited work on inverse problems. The main challenges related to inverse problems for reaction-diffusion systems are the need to store the time-history of the solution, to compute adjoints, and to invert the reduced Hessian, a nearly compact operator. To address these challenges, we have developed two novel methods: a special-purpose multigrid preconditioner and a massively- parallel octree-based meshing algorithm. Multigrid addresses the inversion operator complexity. Octree meshing addresses the efficient construction of highly non-uniform spatial discretizations, which are necessary for reactive-diffusive systems. The algorithms enable us to solve new classes of previously-intractable inverse problems, and, in particular, cardiac electrophysiology.

Reaction-diffusion PDEs are effective models for many important problems in science and engineering. Examples include intracellular signaling, growth of bacterial colonies and tumors, cardiac electrical activity, crystal growth, combustion and radiation, self-assembly, and dislocation and impurity aggregation in crystalline materials. Such systems often exhibit strong, chaotic behavior, and a large range of scales.

Systematic parameter estimation and controllability technologies tailored to such systems have the potential for scientific and technological breakthroughs. For example, it is known that spatial inhomogeneity of diffusive or reaction properties can interfere with pattern formation which in turn can accelerate or terminate a self-assembly process. Is it possible to design the diffusive properties in order to achieve given patterns? Changing the spatial reaction kinetics coefficients (as in ischemic tissue) can cause disruption of electric potential propagation and thus lead to fibrillation and sudden death. Is it possible to predict such failures? Is it possible to match canonical physiological models to patient specific information? We have developed two technologies that enable the solution of such problems: multigrid solvers, and octree data-structures. *These methods enable us, for the first time, to construct ischemic tissue maps of the myocardium, based on multi-lead ECG-data and partial (in vivo) measurements of the action potential on the endocardium.*

We have designed a **multigrid algorithm** such inverse problems. The main feature of the method is that it is mesh-independent even in the case of zero regularization (when the data is in the range of the inversion operator). This makes the method algorithmically robust to the value of the regularization parameter. The method is based on a reduced space formulation in which

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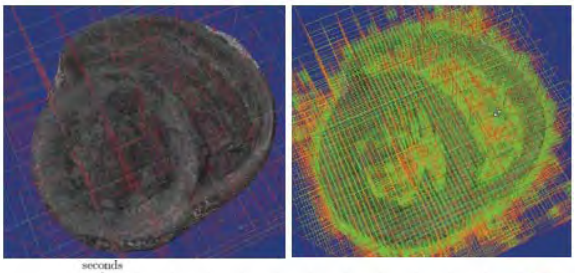
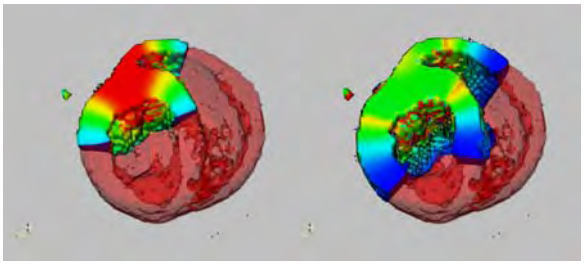
we iterate in the inversion parameter space. We use a full multigrid scheme with a spectrally filtered stationary approximate-Hessian stationary smoother and standard intergrid transfer operators. For constant-coefficient problems the method is provably optimal. We have observed mesh-independent convergence factors resulting in O(N) complexity, where N is the number of state variables. We also discuss the overall multigrid by using a 2-step iterative smoother, and Fourier transforms to do the inter-grid transfers. We have shown that this scheme is extends to nonlinear reaction problems. *This new technology makes feasible the solution of very large scale inverse problems involving millions of unknown parameters.*

Octree-based meshing is used in solving large scale partial differential equations with variable coefficients. It offers both the flexibility of unstructured meshing and the simplicity of Cartesian grids. We have developed new parallel algorithms for the construction and 2:1 balance refinement of large linear octrees and using them for the construction of conforming, second-order accurate, trilinear finite element discretizations on distributed-memory machines. We use several techniques to minimize overhead: a novel bottom-up tree-construction and 2:1 balance constraint enforcement; a three fold compression in the representations for the element connectivity and the octree amounting to a total of 4 words per octant; overlapping communication and computation; and byte alignment for cache efficiency. t element. The cost of applying the Laplacian is comparable to that of applying it using a direct indexing regular grid discretization with the same number of elements. *Our algorithm has scaled up to four billion octants on 4096 processors on a Cray XT3 at the Pittsburgh Supercomputing Center. The overall tree construction time is under a minute—in contrast to previous implementations that required several minutes.*

Novel multigrid methods and octree-based discretizations in cardiac electrophysiology. *Top*: Coarse and fine discretizations of the ventricles of a human heart. *Center*: Scalability analysis of the non-uniform meshing *Bottom*: 2-species model of the propagation of the electric action potential in the heart.



Octree Construction	0.99	1.41	1.32	1.40	1.44	1.60	1.51	1.65	1.72	1.75	2.17	2.92	6.68
Octree Balancing	5.34	8.39	8.75	10.55	11.94	12.57	13.52	13.62	14.67	15.99	18.53	25.42	34.44
Meshing	16.01	23.57	23.19	25.15	26.77	28.99	27.03	29.52	34.91	35.56	36.63	38.23	41.14
MatVec (5)	18.61	20.72	21.09	20.59	23.29	27.79	25.78	27.65	33.01	31.12	32.40	33.24	28.27
Points	180K	361K	720K	1.47M	2.89M	5.8M	11.7M	23.5M	47M	94M	188M	376M	752M
Unbalanced Octants	607K	1.2M	2.4M	4.9M	9.7M	19.6M	39.3M	79.3M	158M	315M	635M	1.26B	2.52B
Balanced Octants	996K	2M	4M	8M	16M	31.9M	64.4M	131M	257M	519M	1.04B	2.05B	4.16B
Independent Vertices	660K	1.3M	2.7M	5.2M	10.5M	21.5M	42M	87.8M	172M	399M	702M	1.36B	2.72B



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