

Titles and Abstracts  
of the Poster Presentations  
for the  
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Metric-induced wrinkling of an elastic thin film  
and  
Wrinkles as a relaxation of compressive stresses  
in annular thin films

Peter Bella

April 7, 2011

**Abstract**

We study the wrinkling of a thin elastic sheet caused by a prescribed non-Euclidean metric. This is a model problem for the folding patterns seen, e.g., in torn plastic membranes and the leaves of plants. Following the lead of other authors we adopt a variational viewpoint, according to which the wrinkling is driven by minimization of an elastic energy subject to appropriate constraints and boundary conditions. Our main goal is to identify the scaling law of the minimum energy as the thickness of the sheet tends to zero. This requires proving an upper bound and a lower bound that scale the same way. The upper bound is relatively easy, since nature gives us a hint. The lower bound is more subtle, since it must be ansatz-free.

**Abstract**

It is well known that elastic sheets loaded in tension will wrinkle, with the length scale of wrinkles tending to zero with vanishing thickness of the sheet [Cerde and Mahadevan, *Phys. Rev. Lett.* 90, 074302 (2003)]. We give the first mathematically rigorous analysis of such a problem. Since our methods require an explicit understanding of the underlying (convex) relaxed problem, we focus on the wrinkling of an annular sheet loaded in the radial direction [Davidovitch et al, arxiv 2010]. While our analysis is for that particular problem, our variational viewpoint should be useful more generally. Our main achievement is identification of the scaling law of the minimum energy as the thickness of the sheet tends to zero. This requires proving an upper bound and a lower bound that scale the same way. We prove both bounds first in a simplified Kirchhoff-Love setting and then in the nonlinear three-dimensional setting. To obtain the optimal upper bound, we need to adjust a naive construction (one family of wrinkles superimposed on the planar deformation) by introducing cascades of wrinkles.

# Nodal Sets of Stekloff Eigenfunctions

Katarína Bellová

April 8, 2011

## Abstract

We study the nodal sets of Stekloff eigenfunctions, i. e. solutions of  $\Delta u = 0$  in  $\Omega$ ,  $\frac{\partial u}{\partial \nu} = \lambda u$  on  $\partial\Omega$ , where  $\Omega$  is a sufficiently smooth domain in  $\mathbb{R}^n$ . Our goal is to estimate the Hausdorff  $(n - 2)$ -dimensional measure of the nodal set on the boundary,  $\mathcal{H}^{n-2}(\{x \in \partial\Omega : u(x) = 0\})$ , in terms of the eigenvalue  $\lambda$ . In case that  $\Omega$  is an analytic domain, we aim for a polynomial bound in  $\lambda$ . The non-analytic case is more subtle and requires the use of additional compactness methods, by which we only get a non-explicit bound.

Our main tool is a generalization of the frequency  $N(r) = r \int_{B_r(a)} |\nabla u|^2 / \int_{\partial B_r(a)} u^2$ . We use the monotonicity of  $N$ , and show a doubling property  $\|u\|_{L^2(B_{2R}(a) \cap \partial\Omega)} \leq C(N) \|u\|_{L^2(B_R(a) \cap \partial\Omega)}$  for  $a \in \partial\Omega$ .

This is a work in progress.

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Title: Topological specificity in cytokine response coding

A calibrated host response to microbial pathogens requires the production of both pro-inflammatory cytokines like interleukin-6 (IL-6) and anti-inflammatory cytokines, such as interleukin-10 (IL-10). This balance is crucial for successful resolution of microbial infection, as insufficient inflammatory cytokine production can result in inadequate control of pathogens, while excessive inflammation can lead to autoimmune injury or a toxic cytokine storm. However, it is unclear how numerous cytokines can code for a large number of specific responses using relatively few signaling pathways. IL-6 and IL-10, for example, both signal through the JAK/STAT3 pathway, but ultimately produce very different cellular responses. In each case, the cytokine binds to its cognate receptor, leading to STAT3 phosphorylation, nuclear localization, and subsequent gene activation.

An important distinction between the two signaling systems is that while SOCS3 is produced by both cytokines, it only exerts its inhibitory effect downstream of IL-6 signaling. Our initial studies suggest that the distinct IL-6 and IL-10 network topologies confer response specificity by altering the activation dynamics of STAT3. We integrated single-cell response time course experiments and computational modeling to investigate the role of network topology in controlling the dynamics of STAT3 activation and the corresponding cellular responses in human dendritic cells (DCs). A differential equation model, multispectral flow cytometry, and high-resolution imaging flow cytometry all indicate that IL-6 stimulation results in a transient activation of STAT3, with a decline in phosphorylation and nuclear localization corresponding to the production of the feedback inhibitor SOCS3. In contrast, IL-10 signaling resulted in sustained STAT3 activation. Further, truncation of IL-10 signaling using receptor-neutralizing antibodies resulted in transient STAT3 phosphorylation and led to an IL-6—like gene response, suggesting that the dynamics of STAT3 activation direct the cellular response. Stochastic modeling of these two signaling systems further provided a mechanistic interpretation consonant with experimental data and will be used to generate predictions to guide subsequent experimentation. Ultimately, the distinct IL-6 and IL-10 signaling network topologies confer specificity in the cellular response by controlling duration of STAT3 activation. This line of investigation may help explain the basis for a fundamental immune response signaling question: how do multiple receptor systems regulate identical signal components to generate diverse and specific cellular responses.

Evan Chou, Math PhD student

Title: A Multiscale Approach to Digital Halftoning

Abstract:

We present ongoing research concerning a particular multiscale approach to digital halftoning. Digital halftoning is the process of rounding values in an interval  $x_i \in [0,1]$  to the endpoints  $q_i \in \{0,1\}$  so that the error  $x - q$  with respect to some measure is minimized. In our approach, we construct a tree from the image, where each level is an averaging of the finer level. We then "round" this tree, starting from the coarsest level at the top, and working back down to the finest level at the bottom, taking steps to ensure that at the bottom level we obtain a valid rounding. We start with a simple case, using a Haar average over disjoint values, and then we look to find ways to work with more complicated averages.

Naftali Cohen, CAOS PhD student

Title: A Modeling Framework to Study Interaction between Resolved and Parameterized Waves

We present an idealized Atmospheric General Circulation Model (AGCM) designed to explore the interactions between parameterized gravity waves and the resolved circulation. The model is based on an AGCM used in recent studies to explore coupling between the stratosphere and troposphere. In the earlier model, the effect of gravity waves on the stratospheric circulation was parameterized as Rayleigh friction near the model lid, which can lead to physically inconsistent circulations that do not conserve momentum. This crude parameterization is replaced with orographic and non-orographic gravity wave parameterizations which are similar to those used in state-of-the-art coupled climate models. We first verify that the main results from the model with Rayleigh friction are robust: a strengthened polar vortex in the stratosphere leads to a poleward shift in the tropospheric jet stream, both for climatological changes in the stratospheric forcing and for natural variations of the vortex. We then focus on the coupling between parameterized gravity waves and resolved planetary waves during Stratospheric Sudden Warming events, comparing the model with recent observational estimates of gravity wave activity during sudden warmings.

# Object detection, image segmentation and scenes parsing using convolutional network

Benoit Corda, Clément Farabet and Yann LeCun

Computation and Biological Learning Lab, NYU

Scene parsing is the task of assigning a class label to each pixel of an image. Although very similar to image segmentation, the scene parsing requires an understanding of high-level relationship between objects appearing on the scene. Whereas the segmentation goal is to create cluster of pixels that belongs to the same object. The scene parsing not only needs to groups similar things together, but also must recognize the category of the groups and understand their spatial dependencies.

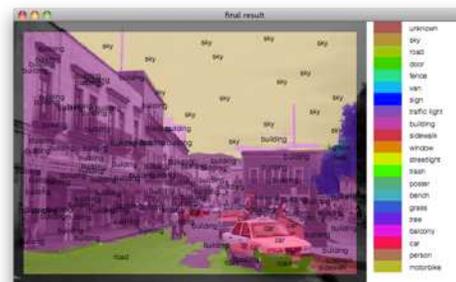
Here we propose an inference model based on convolutional neural network for scene parsing. The power of this approach has two fold, at the same time the model can provide an object detection system and an image segmentation of the input image.

Inspired by previous work from Grangier et al.<sup>[1]</sup>, we used a subset of the LabelMe dataset (<http://people.csail.mit.edu/torralba/benchmarks/>) that contains about 3000 images of spanish cities to train our model and we removed 10% of the set for validation. From the thousand classes we kept the twenty most frequent and merge the objects that were conceptually similar (e.g. car and truck). All the images were first resized to  $500 \times 375$ , then 400 million patches were randomly sampled to produce a  $20 \times 1e8 \times N \times N$  tensor where the first dimension indexes the classes, the second indexes patches of which the center pixel belongs to the corresponding class, and the last two dimensions are the height and width of the patch.

The training is done in a greedy fashion using stochastic gradient descent (SGD). First we used a model called CN1 similar to LeNet-5<sup>[2]</sup> with 3 convolutional layers with small filters (5x5). After convergence we increase the size of the filters to 9x9 (model CN2), and finally we add a fourth convolutional layer with the same filter size 9x9 (model CN3). With this protocol, we managed to get our best model to reach more than 72% of pixel accuracy (cf. example below).



Street scene that the model never saw before.



Output of the model's classification

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[1] D. Grangier, L. Bottou, and R. Collobert. Deep convolutional networks for scene parsing. ICML 2009 Deep Learning Workshop, June 2009

[2] Y. LeCun, F.-J. Huang, and L. Bottou. Learning methods for generic object recognition with invariance to pose and lighting. In Proceedings of CVPR'04. IEEE Press, 2004

Edoardo Corona, Math PhD student

Title: Inextensible vesicle evolution in the presence of smooth boundaries

Abstract:

On this research project with Denis Zorin and Shravan Veerapareni<sup>1</sup>, the goal is to simulate the flow of inextensible vesicles (Stokes flow) in the presence of walls or boundaries. At each time step, we are using Lexing Ying's  $O(N^{3/2})$  fast boundary integral solver<sup>2</sup> to enforce the no slip boundary condition on a smooth, solid object of arbitrary geometry. For this purpose, it was necessary to write a number of routines using MEX to communicate between Matlab and C++.

Our first tests will be presented, including a simple example in which we drive an inextensible vesicle towards a solid sphere under a background shear flow. Aggressive smoothing and re-parametrization are often required to avoid numerical instability. Our short term goal is to perform a series of experiments to study the physics of different vesicle flows, such as flow through in a torus with a narrow section and flow in porous media. Ultimately, our aim is to extend the work of George Biros and Denis Zorin and simulate the flow of a considerable number of vesicles in the presence of physical boundaries (such as a blood vessel wall). Some of the challenges that we expect include an increase in numerical stiffness as vesicles approach walls and including collision detection methods.

This is also one of the applications which motivates our ongoing work on fast direct solvers for integral equations in three dimensions.

<sup>1</sup> S. Veerapareni, A. Rahimian, G. Biros, D. Zorin, "A fast algorithm for simulating vesicle flows in three dimensions" \*

<sup>2</sup> L. Ying, G. Biros, D. Zorin, "A High Order 3D Boundary Integral Equation Solver for elliptic PDEs in smooth domains" \*Journal of Computational Physics 219, 1, (2006) pp. 247-275\* \*

Dharshi Devendran, Math PhD student

Title: An Immersed Boundary Energy-Based Method for Incompressible Viscoelasticity

We present a method for incompressible viscoelasticity which does not use stress tensors and in which Lagrangian (material) coordinates are used to describe elastic forces, and Eulerian (spatial) coordinates are used for the equations of motion and incompressibility condition. The elastic forces are computed directly from an energy functional and the immersed boundary method is used to communicate between Lagrangian and Eulerian variables. The method is applied to a warm-up problem, in which a viscoelastic incompressible material fills a two-dimensional periodic domain. For this problem, we study convergence of the velocity field, the deformation map, and the Eulerian force density. The numerical results suggest that the velocity field and deformation map converge strongly at second order and the Eulerian force density converges weakly at second order. Incompressibility is well maintained, as indicated by area conservation in this 2D problem. Finally, the method is applied to a three-dimensional fluid-structure interaction problem.

Thomas Fai, Math PhD student

Title: An FFT-based Immersed Boundary Method for Variable Viscosity and Density Fluids

Abstract:

The immersed boundary (IB) method is a general numerical method for simulating fluid-structure interaction. In the past, the IB method was limited to uniform viscosities unless additional techniques were used to keep track of the interfaces between fluid regions. The present method overcomes this difficulty by embedding marker particles in the fluid that "spread" variations in viscosity and density onto the grid and are passively advected. We treat the non-uniform parts explicitly so that FFT's can be used, as in the constant coefficient case but with an adjusted effective forcing term. Empirical convergence rates, which show second-order convergence for sufficiently smooth problems, will be presented. Red blood cells and heterogeneous flows through pipes are among possible applications of this method. Our preliminary simulations will be discussed.

Pau Gazzillo, C.S. PhD

Title: Syntactic Foundations for Refactoring C Or: How to Tame the C Preprocessor

Software refactoring tools are becoming indispensable by replacing repetitive and error-prone editing tasks with automated and correct source code transformations. Yet, complete refactoring support for C is difficult to achieve. First, refactoring tools need to handle *two* languages at the same time: the actual C language and the C preprocessor. Second, the preprocessor is a textual substitution system and operates at the level of individual tokens. Unfortunately, existing refactoring tools punt on the full complexity of processing these two languages. They assume that preprocessor usage is well-formed, i.e., preserves C's syntactic units (expressions, statements, and so on) and/or that code has only a single configuration (no conditionals). Yet both assumptions break even for familiar headers such as "stdio.h".

To enable refactoring C in the presence of almost all preprocessor (ab)use, this paper explores two complementary techniques: Normalization significantly simplifies the implementation of refactoring tools and denormalization restores the original sources modulo desired changes. As explained in this paper, normalization entails expanding macros across all configurations, so that tokens have their apparent C language meaning. More importantly, it entails using a new variant of LR parsing to rewrite conditionals. This results in conditionals bracketing only complete syntactic units and facilitates their treatment as just another language construct. Finally, it entails careful optimizations to limit the state space explosion faced by any preprocessor normalization scheme. Denormalization then undoes both macro expansion and conditional rewriting based on annotations collected during normalization. We describe these techniques in detail and present a Java-based tool, which successfully processes the entire Linux kernel including all conditional code. Overall, we lay the syntactic foundations not only for refactoring C, but also analyzing and translating C across all configurations at the same time.

Maria Gehne, AOS PhD student,

Title:

Spectral analysis of tropical atmospheric dynamical variables using a linear shallow water modal decomposition

Abstract

Space-time spectral analysis has been used frequently in studying observational evidence of convectively coupled equatorial waves. Here 20 years of brightness temperature data (Tb) and dynamical reanalysis data are analyzed by an appropriate projection onto the meridional basis functions of the beta-plane linear shallow water equations. Evidence of peaks in power along linear equatorial mode dispersion curves in Tb, zonal and meridional wind, divergence and geopotential spectra are presented. The main feature of all space-time spectra considered is the redness in frequency, zonal wave number and meridional mode number. It is found that spectral peaks in the dynamical variables spectra are largely consistent with linear shallow water theory, but spectral peaks related to barotropic waves and extratropical storm track activity are apparent as well. The convectively coupled wave signals are seen to be confined to the first few meridional basis functions suggesting a possibility for reducing noise when filtering for these signals and implications for future modeling work. A comparison of our results for two different reanalysis products shows only minor differences adding confidence in the robustness of the analysis presented. This emphasizes the fact that any comprehensive theory of tropical convection should explain both this ubiquitous (and robust) redness as well as the marked presence of linear waves within tropical variability.

Carl Gladish, AOS PhD student

Title: Modeling the mechanics and thermodynamics of ice shelves in warm oceans

Ice shelves are the floating ice masses at the interface between polar ice sheets and the surrounding oceans. Often ice shelves are buffered from warmer water masses by a layer of water very near the freezing point. In some cases, however, such as Pine Island Glacier in Antarctica and Petermann Glacier in Greenland, ice shelves are in direct contact with relatively warm water and as a consequence they experience rapid melting and undergo a unique dynamical response. We present numerical model results that explore the poorly-observed dynamics of this ice and ocean system. In particular, we model the channelization of basal melting at the ice-shelf/ocean interface and the resulting stress fields which may account for the unique ice morphology of these glaciers.

Sara Grundel, Math PhD student

Title: A rational subdivision sphere

It is a well known advantage of NURBS over subdivision surfaces that it can reproduce conic sections. The advantage of subdivision is that it can reproduce arbitrary topology. We explore the representation of the sphere as rational subdivision surface coming from a newly developed subdivision scheme that is  $C^2$  smooth everywhere. With a relatively coarse mesh we can describe the sphere in this setting.

# AN ANALYSIS OF THE CRITICAL POINTS OF THE PROPELLER PROBLEM

STEVEN HEILMAN, AUKOSH JAGANNATH, AND ASSAF NAOR

ABSTRACT. After proving a generalization of the semidefinite Grothendieck inequality, Khot and Naor conjectured a value for the inequality's optimal constant. These authors also reduced the calculation of this constant to a finite dimensional geometric optimization problem. For the first nontrivial case, we prove this conjecture by reducing to an isoperimetric problem on the sphere and then using a numerical computation.

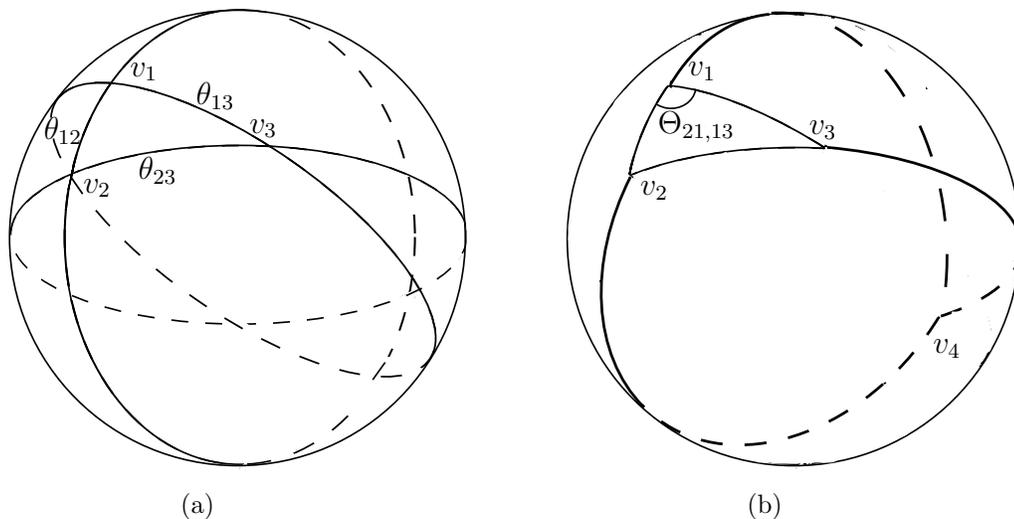


FIGURE 0.1. (a) Spherical triangle constructed with three great circles (b) Partition of the sphere into four spherical triangles. We need to optimize the sum of the squared lengths of a partition as shown.

{fig1}

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An-Sheng Jhang, Math PhD student

Title: Growing Suspensions

Abstract:

We study the kinetic representation of growing rod suspensions. Coupled with Stokes equation, we can use Fokker-Planck equation to describe the evolution of density. The main difference of this study from previous study about swimming body is that growing rod suspensions don't self-propel but still contribute to stress due to growing. With theory and numerical experiment, we showed that despite they are only growing, there is still a phase-transition condition such that it would deviate from isotropic state and produces complex flows. We also studied other instabilities and properties of the induced flow.

# FAST DIRECT SOLVERS BY MULTILEVEL MATRIX COMPRESSION

KENNETH L. HO

We present a fast direct solver for structured linear systems based on the hierarchical application of the interpolative decomposition. The structure imposed on the system matrix is that, up to permutation, there is a block tree on the rows and columns such that at each level of the tree, the submatrix corresponding to each row or column block, possibly with the diagonal block deleted, is low-rank. This describes, e.g., Laplace-type ( $1/r$ ) interactions between points in space, sorted according to an octree ordering. We use the interpolative decomposition to recursively compress each block by identifying row or column skeletons, which define a subblock of near-optimal rank from which the entire block can be reconstructed, by merging and compressing the skeletons at the previous level. This multilevel procedure computes a compressed representation of the matrix, which allows for efficient storage, fast matrix-vector multiplication, and fast matrix factorization and inverse application via embedding into a highly structured sparse matrix.

For boundary integral systems with non-oscillatory kernels satisfying Green's identity, e.g., Laplace, Yukawa, or low-frequency Helmholtz, the solver has complexity  $\mathcal{O}(N)$  in 2D and  $\mathcal{O}(N \log N)$  in 3D. As a numerical example, the Laplace potential interaction matrix between  $N = 2^{17} = 131072$  charges equispaced on the unit circle can be compressed to nine digits in 13 s on a modern laptop, applied in 0.07 s, factored in 7 s, and its inverse applied in 0.1 s. Ignoring precomputation, the solution time is more than an order of magnitude less than that of fast iterative methods based on, e.g., GMRES driven by fast matrix-vector products using the FMM.

We expect our work to apply widely to many problems in science and engineering, particularly in solving systems with singular geometries, simulating dynamics in fixed domains, or in the context of design, where many similar systems must be solved.

This is joint work with Leslie Greengard and Zydrunas Gimbutas.

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# Automated Detection of Diabetic Retinopathy using an Artificial Neural Network

Angjoo Kim, Rob Fergus, Nathan Silberman

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Diabetic retinopathy, the most common eye disorder caused by diabetes, is the primary cause of blindness in America and over 99% of cases in India. It is caused by changes in the blood vessels of the retina, where sometimes blood vessels may swell, leak fluid, and block vision. Unfortunately there is no known cure for diabetic retinopathy and early detection of the disease is essential in preventing blindness.

The purpose of this study was to extend the existing work in developing an automated detection system for diabetic retinopathy. Initial efforts towards building such a system used a range of computer vision techniques along with a Support Vector Machine (SVM) classifier trained to recognize indicators of retinopathy in retinal images.

This study used an Artificial Neural Network (ANN) classifier instead of the SVM classifier in hopes of improving the performance of the system. An ANN with back propagation was implemented and trained to recognize exudates, bright yellow spots of fat deposits in the retina, which in turn lead to blood clots and spillage. The training set consisted of SIFT features obtained from 33 retinal images with pixel-level labels marked by ophthalmologists at NYU.

The effects of different methods of selecting training features and different network variables were assessed. The current accuracy of the ANN classifier does not improve that of the SVM classifier. However, there are immediate improvements in the training process and evaluation of the classified data that could potentially improve the overall accuracy the system with a neural network.

## **Glucose Regulation in Diabetes**

*Samantha Lozada, Mathematics*

*Mentors: Dr. Charles S. Peskin, Mathematics*

*Thomas Fai, Mathematics*

Complicated and extensive models of glucose regulation, involving several variables, have been developed over the years. Our research specifically focuses on the feedback loop between insulin and glucagon. Although our model is simpler than a model including state variables such as non-esterified fatty acids concentration in the blood plasma,  $\beta$ -cell mass, TAG content of lipocytes, and/or leptin concentrations in the blood plasma, we are still able to simulate most of the key effects of diabetes and other health problems on glucose regulation; such as, hyperglycemia, hyperinsulinism, and insulin shock (hypoglycemia). We are even able to simulate eating a bowl of vanilla ice cream!

Enkeleida Lushi, Math PhD student

Title: Chemotaxis in Suspensions of Micro-swimmers

Suspensions of self-propelled particles and microorganisms are known to exhibit complex dynamics as a result of hydrodynamic interactions as well as responses to chemical cues or nutrients in a process known as chemotaxis. Such active suspensions are found in nature, where bacteria are known to organize in large-scale colonies and can show correlated motions due to both hydrodynamic and chemical interactions. Chemotaxis has been exploited to make biological swimmers perform specific technological tasks, such as enhancing fluid mixing in microfluidic systems, and recently developed synthetic swimmers that exhibit chemotactic effects can be used for drug delivery in the body. The goal of our project is to develop and analyze a model that fully couples chemotactic responses and hydrodynamic interactions in active suspensions.

We develop a kinetic theory and use nonlinear continuum simulations to study run-and-tumble chemotaxis in the collective dynamics of self-propelled particle suspensions. The stability of isotropic suspensions is analyzed to show an instability and growth of fluctuations due to chemotaxis, for Pusher (rear-actuated microswimmers such as bacteria) and Puller (front-actuated swimmers like some microalgae) particles alike. Using full nonlinear simulations, we investigate the long-time dynamics of chemotactic suspensions and observe growth in density fluctuations for both Pullers and Pushers. In Pusher suspensions, where strong density fluctuations are known to develop due to hydrodynamics, chemotaxis affects these fluctuations and enhances the fluid mixing.

Andrew Matteson, COB PhD student

Title: Model Merging and Parameter Identification of EGFR and c-MET Signaling Cascades

Epidermal growth factor receptor (EGFR) is a receptor tyrosine kinase (RTK) commonly over expressed in epithelial cancers. Targeted therapies have been developed to treat cancers that over express EGFR, but they have had limited success. The full potential of EGFR targeted therapies has been hindered primarily by a variety of innate and acquired resistance mechanisms to the treatments. Disregulation of mesenchymal epithelial transition factor (MET), an RTK associated with angiogenesis and wound healing, has been proposed as a possible mediator of targeted therapy resistance.

In an effort to understand interactions between the two RTKs, we are currently seeking a mechanistic model that can predict signaling in response to stimulation from EGF and HGF, ligands of EGFR and MET respectively, administered alone or in combination across a range of doses with and without the presence of inhibitors.

A validated model with these features would assist in identification of potential therapeutic synergies and in biomarker discovery.

Here we present progress in the development of an EGFR-cMET model under stimulation by EGF and HGF validated against phosphorylation responses of both receptors and ERK (a proliferation and survival factor in cancer). Specifically, we have a single model that predicts signaling over the course of two hours in response to stimulation by EGF or HGF alone with high accuracy across a range of ligand doses.

ERK signaling in ACHN cells in response to high concentrations of both HGF and EGF is suppressed relative to the high dose, single ligand cases. This was an unanticipated result reproduced by the model under costimulation in a qualitative way. The model suggests inhibition by high doses of both ligands is caused by combinations of multiple functional roles of GAB1.

The poster will give special attention to issues related to model merging and parameter identification.

# Two-dimensional slope limiting for embedded boundary grids

Sandra May

Many two-dimensional, second-order accurate finite volume methods are based on the following 3 steps:

1. Construct a (limited) linear polynomial in every cell out of the given cell averages ( $u_{ij}^n$ ).
2. Calculate the fluxes through the cell edges using the linear polynomial.
3. Update the cell averages to ( $u_{ij}^{n+1}$ ) using the fluxes through the edges.

In Step 1, a limiter is needed which adjusts the slope appropriately. The limiter prevents overshoots and oscillations that arise at discontinuities, as well as maintaining positivity, since for example if pressure becomes negative your code will crash. Limiters in one dimension are very well understood, see e.g. the paper by Sweby [Swe84]. In two dimensions for rectangular grids a one-dimensional limiter is usually applied in the  $x$  and  $y$  direction separately. This approach is very straightforward to realize and usually works well. However, this splitting of  $x$  and  $y$  components of the gradient relies on the cell edges being aligned with the coordinate axes.

On non-rectangular grids a two-dimensional limiter is much more difficult to realize – especially for embedded boundary grids with ‘cut cells’, the motivation for this work. By ‘cut cell’ we refer to the cells which arise around the boundary of a solid object which is cut out of a background Cartesian grid. These cells vary considerably in terms of size and structure. The standard approach for these cells, or more generally for unstructured meshes, uses a scalar limiter, where the  $x$  and  $y$  components are decreased by a scalar until there are no overshoots (possibly the scalar is zero). Our approach for limiting is based on the work by Berger, Aftosmis, and Murman [BAM05]. There, the authors develop the idea of formulating the limiter as an optimization problem: retain as much of the unlimited gradient as possible while fulfilling some monotonicity conditions in order to avoid overshoot. This allows us to use different scaling factors for the  $x$  and  $y$  components of the gradient in order to minimize diffusion.

We have worked on different formulations for the objective function and the constraints as well as on different ways to solve the resulting optimization problem. We currently formulate this as a linear programming problem and use the all-inequality Simplex method for its solution. We show results where the error using our new limiter compared to using a scalar limiter has been reduced significantly. We are currently working on additional test problems as well as extensions to three dimensions. We will also test our limiter on general unstructured grids.

## References

- [BAM05] M. Berger, M. J. Aftosmis, and S. M. Murman. Analysis of slope limiters on irregular grids. In *43rd AIAA Aerospace Sciences Meeting, Reno, NV*, 2005. Paper AIAA 2005-0490.
- [Swe84] R. K. Sweby. High resolution schemes using flux limiters for hyperbolic conservation laws. *SIAM J. Numer. Anal.*, 21:995–1011, 1984.

# Scoring-and-Unfolding Trimmed Tree Assembler: Algorithms for Assembling Genome Sequences Accurately and Efficiently

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Aprile 2011

## Abstract

Mired by its connection to a well known  $\mathcal{NP}$ -complete combinatorial optimization problem — namely, the Shortest Common Superstring Problem (SCSP) — historically, the whole-genome sequence assembly (WGSA) problem has been assumed to be amenable only to greedy and heuristic methods. By placing efficiency as their first priority, these methods opted to rely only on local searches, and are thus inherently approximate, ambiguous or error-prone, especially, for genomes with complex structures. Furthermore, since choice of the best heuristics depended critically on the properties/errors of the input data and the available long range information, these approaches hindered designing an error free WGSA pipeline.

We dispense with the idea of limiting the solutions to just the approximated ones, and instead favor an approach that could potentially lead to an exhaustive (exponential-time) search of all possible layouts. Its computational complexity thus must be tamed through a constrained search (Branch-and-Bound) and quick identification and pruning of implausible overlays. For his purpose, such a method necessarily relies on a set of score-functions (*oracles*) that can combine different structural properties (e.g., transitivity, coverage, physical maps, etc.). We give a detailed description of this novel assembly framework, referred to as SUTTA (Scoring-and-Unfolding Trimmed Tree Assembler), and present experimental results on several bacterial genomes using next generation sequencing technology data.

## References

- [1] Giuseppe Narzisi and Bud Mishra. Scoring-and-Unfolding Trimmed Tree Assembler: Concepts, Constructs and Comparisons. *Bioinformatics*, Oxford Journals, (2011) 27 (2): 153-160.

Andras Pataki, Math PhD student

Title: High order methods for computing axisymmetric plasma equilibria

Abstract:

We present a high order numerical method for computing equilibria of axisymmetric plasmas solving the Grad-Shafranov equation of ideal MHD. Current solvers typically use finite element or finite difference methods, and have difficulties calculating derivatives with high-order accuracy. This is due, in part, to the need for one-sided approximations near the domain boundary and, in part, to the cancellation errors inherent in numerical differentiation. Our solver aims to eliminate these difficulties by using a mix of integral equation and spectral methods, and thus can calculate all first and second derivatives with the same high convergence rate without the need for additional grid points. In brief, a change of variables is used to transform the leading differential operator into the standard two dimensional Laplacian. A conformal map is then constructed to pose the problem as a Poisson problem in the unit disk, where a fast spectral solver based on separation of variables is applied. Since most interesting equilibrium calculations involve a nonlinear plasma profile and require an eigenvalue computation, a nonlinear outer iteration is used to arrive at the final solution. We have successfully demonstrated the procedure for ITER-like and spherical tokamak plasma profiles and typically achieve 10+ digit accuracy in the solution and its derivatives in under a minute on single CPU core on a 512 by 512 grid.

# Principal components: a descent algorithm.

Rebeca Salas–Boni and Esteban G. Tabak

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A descent algorithm is developed for the calculation of principal components and, more generally, for the search of low-dimensional subspaces of a high-dimensional vector space satisfying an optimality property. The algorithm minimizes the cost function through a series of orthogonal rotations, each represented economically as the exponential of a skew-symmetric matrix picked from a comparatively small-dimensional manifold. We study two different ways of choosing this matrix: One, using gradient descent. The second one is using second-order descent, where the special structure of our cost function allows us to approximate iteratively the solution of the system determined by Newton’s method. The performance of the algorithm presented is illustrated via several numerical examples, some synthetic and one using oceanographic data. This is joint work with my advisor, E. G. Tabak.

# Traffic Signs and Pedestrians Vision with Multi-Scale Convolutional Networks

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Convolutional Networks (ConvNets) are biologically-inspired multi-stage architectures that automatically learn hierarchies of invariant features. While many popular vision approaches use hand-crafted features such as HOG or SIFT, ConvNets learn features at every levels from data that are tuned to the task at hand. The traditional ConvNet architecture was modified by feeding 1st stage features in addition to 2nd stage features to the classifier (Fig 1). We apply these multi-scale ConvNets to the tasks of traffic sign classification (Fig 2) and pedestrian detection and establish new accuracy records, above human performance for road signs. We also show a significant accuracy gain on the pedestrian task when using unsupervised pre-training with Convolutional Predictive Sparse Coding [1] (ConvPSD). The ConvNet was implemented using the EBLearn C++ open-source package <sup>1</sup>.

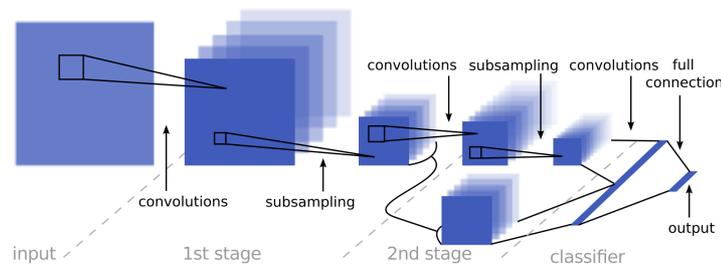


Figure 1: A 2-stage multi-scale ConvNet architecture. The input is processed in a feed-forward manner through two stage of convolutions and subsampling, and finally classified with a linear classifier. The output of the 1st stage is also fed directly to the classifier as higher-scale features.



#	Team	Method	Accuracy
	<b>sermanet</b>	<b>EBLearn 2LConvNet ms 108 feats + 100-feats CF classifier + No color</b>	<b>99.17%</b>
197	IDSIA	cnn_hog3	98.98%
196	IDSIA	cnn_cnn_hog3	98.98%
<b>178</b>	<b>sermanet</b>	<b>EBLearn 2LConvNet ms 108 feats</b>	<b>98.97%</b>
195	IDSIA	cnn_cnn_hog3_haar	98.97%
<b>187</b>	<b>sermanet</b>	<b>EBLearn 2LConvNet ms 108 + val</b>	<b>98.89%</b>
199	INI-RTCV	Human performance	98.81%
170	IDSIA	CNN(IMG)_MLP(HOG3)	98.79%

Figure 2: **Left:** Difficult road sign examples in GTSRB coming from real-word perturbations. **Right:** Official top 7 results and new accuracy record after GTSRB Phase 1 (99.17%).

## References

- [1] Kavukcuoglu, K, Sermanet, P, Boureau, Y, Gregor, K, Mathieu, M, and LeCun, Y. Learning convolutional feature hierachies for visual recognition. In *Advances in Neural Information Processing Systems (NIPS 2010)*, 2010.

<sup>1</sup><http://eblearn.sf.net>

## ***The Aging Mechanism of Soman inhibited Acetylcholinesterase***

Gulseher Sarah Sirin, Yingkai Zhang

Acetylcholinesterase (AChE) is a serine hydrolase localized to the cholinergic synapses. Under normal physiological conditions, AChE catalyzes the hydrolysis of neurotransmitter acetylcholine, terminating synaptic transmission.

Organophosphate (OP) compounds such as nerve agents as well as insecticides irreversibly inhibit AChE and result in neuromuscular paralysis and eventual death by asphyxiation. Current search for reactivating agents of inhibited AChEs are based on known oxime compounds with limited reactivating potentials since known oximes can not reactivate AChEs once the bound OPs undergo a dealkylation reaction (aging). All-atom molecular dynamics simulations of non-aged Soman (pinacolylmethylphosphonofluoridate) inhibited AChE were carried out to study the influence of catalytic gorge residues on soman coordination within the active site. Furthermore, the mechanism of Soman-AChE aging was studied using Born-Oppenheimer Ab initio QM/MM molecular dynamics simulations with umbrella sampling. This method uses first principle description of chemical bond formation and breaking within the native protein environment while taking into effect the influence of protein dynamics on the reaction mechanism. Mechanistic Information that has been revealed by this study would be used to find novel compounds capable of reactivating aged AChEs.

Adam Stinchcombe, Math PhD student, Applied Math Lab

Title: Recoil Locomotion at Sea and on Land

Abstract: Recoil is the reaction force, from Newton's Third Law, that a system experiences as one of its components is accelerated. If a body has an internal oscillating mass, it will experience a perpetual recoil. That recoil can be converted into locomotion if the body is exposed to an asymmetrical, dissipative force. One such example is a body in a viscous fluid that varies its shape. Another is a partially submerged body that varies how much it is submerged to create an asymmetry in its viscous drag. An example on land involves a variable friction force timed to impede motion in the "backward" direction and less so in the forward direction. These examples will overturn the common perception that friction hinders locomotion. The behavior in these examples will be analyzed theoretically and illustrated physically with mechanical toys.

Ang Sun, CS PhD student

Title: Semi-supervised Semantic Pattern Discovery with Guidance from Unsupervised Pattern Clusters

Abstract: We present a simple algorithm for clustering semantic patterns based on distributional similarity and use cluster memberships to guide semi-supervised pattern discovery. We apply this approach to the task of relation extraction. The evaluation results demonstrate that our novel bootstrapping procedure significantly outperforms a standard bootstrapping. Most importantly, our algorithm can effectively prevent semantic drift and provide semi-supervised learning with a natural stopping criterion.

Collaborator/advisor: Ralph Grishman

Xichen Li, CAOS PhD student

Title: What will happen if the Solar Radiation reduces by 1/4: Preliminary investigations of the faint young sun paradox using Community Climate System Model.

This is a story of our nascent earth. About 3 billion years ago, while most of the hydrogen had still not been burned in the sun, the solar radiation should be much lower (which is about only 70% of today's level). By energy budget theory, the earth should be covered by thick ice and snow. However, sediment record tell us that there exist a lot of liquid water on the surface that time. An intuitive hypothesis was proposed that increasing the green house gas concentration might keep the earth warm and wet.

However, in this case, the concentration should be a unphysical value... Now paradox arises among the faint sun , the liquid earth, and the green house concentration.

While hypothesis sometime uses a lot of linear approximation, and neglected certain amount of feedbacks, numerical models provide alternative insights into various possible solutions. In this study, a fully coupled climate system model was adopted to simulate the young earth. Sensitivity experiments are designed and we expect the simulation results will offer us some clues or possibilities, or even surprises us just as the real world does.

The poster will present some preliminary results of these experiments and some clues to help solve the paradox.