**Mathematical Sciences Scientific Computing**
**Research Environments (SCREMS)**


## Project Summary

The Department of Mathematics and Statistics at the University of Massachusetts, Amherst proposes to purchase one SGI four-processor machine, one file server, ten X-terminals, a color laser printer, and site licenses for Maple and Matlab which will be dedicated to the support of research for the projects proposed here. We also request funding for partial support for one professional system administrator to setup and maintain this equipment. A specific list of the projects are as follows:

- Computations in Algebraic Geometry: hypergeometric functions, toric varieties, enumerative geometry (Eduardo Cattani, David Cox, Frank Sottile)
- Computational Number Theory: numerical and graphical investigations of Artin $L$-functions (David Hayes, Siman Wong)
- Mesoscopic theories and hybrid computational algorithms in materials science and fluid mechanics (David Horntrop, Markos Katsoulakis, Bruce Turkington)
- Geometry, Computation and Visualization: minimal, constant-mean curvature, and Willmore surfaces in 3 and 4 dimensions (Robert Kusner, Nicholas Schmitt)

The University of Massachusetts, Amherst will contribute cost sharing of 50% of the amount of this purchase, and will assume the full personnel costs after NSF funding ends.

## Project Description

### 1. Overview, and Abstracts of Individual Research Projects

Continuing advances in computer technologies have expanded the opportunities to address an ever widening variety of complex problems in science, engineering and industry, as well as to provide a powerful for discovering and developing new mathematics. The Department of Mathematics and Statistics at the University of Massachusetts, Amherst has a strong tradition in research in computational mathematics, notably geometry (GANG[1]) and applied mathematics. In recent years, researchers in our department have developed and applied computational techniques in algebraic geometry and number theory. The resulting increase in computational activities underscores the demand for additional computational resources within our department. We thus request NSF funding for new equipment and support for new computer facilities.

Below we briefly outline the projects in this proposal.

(i) Computation in Algebraic Geometry (Eduardo Cattani, David Cox, Frank Sottile)

We propose using large-scale symbolic and numerical computation to investigate the important question of real-number solutions to problems of enumerative geometry involving the Schubert calculus. This will help understand a conjecture of Shapiro and Shapiro which has led to important advances in this area. We also propose using symbolic computation to help find Gröbner bases for spaces of curves and toric varieties in Grassmannians and flag manifolds with the goal of obtaining new formulas in enumerative geometry. This may lead to a generalization of quantum cohomology and Gromov-Witten invariants for counting toric subvarieties of these spaces.

(ii) Computational Number Theory (David Hayes, Siman Wong)

We propose to investigate Artin $L$-functions from the numerical and graphical point of view. We will implement a polynomial-time algorithm to compute partial zeta functions of number fields. This allows us to efficiently compute units $p$-adically in connection with the study of Stark conjectures, bypassing the use of functional equations of $L$-functions. We will also study the distribution of values of automorphic forms associated to 2-dimensional complex Galois representations, using the method of color wheels. We expect that such graphical representations will distinguish the dihedral Galois representations from the non-dihedral ones.

(iii) Mesoscopic Theories and Hybrid Computational Algorithms in Materials Science and Fluid Mechanics (David Horntrop, Markos Katsoulakis, Bruce Turkington)

Many important physical problems and industrial processes involve a wide variety of interacting spatial and temporal scales. Here, we propose to develop novel mesoscopic theories that combine features of macroscopic, continuum models with microscopic information in order to study problems in materials science and fluid mechanics. The computational solution of these problems requires the development of new numerical schemes which are intrinsically hybrid in nature, requiring a combination of Monte Carlo and deterministic techniques.

(iv) Geometry, Computation and Visualization (Robert Kusner, Nicholas Schmitt)

The GANG group proposes to continue its path-breaking investigations of minimal, constant mean curvature (CMC) and Willmore surfaces. There has been particularly rapid recent progress constructing and classifying complete CMC surfaces, and determining their moduli spaces, by means of PDE and analytic methods. In the past year a new software tool, `DPWLab` has been developed at GANG. The `DPWLab` software computes and visualizes complete CMC surfaces from meromorphic data; experiments with `DPWLab` are discovering a wealth of new phenomena, and are suggesting new methods for understanding CMC moduli spaces theoretically. We also propose to adapt these software tools to study Willmore surfaces, which is computationally more intensive and will utilize parallelized software on a multiprocessor SGI machine.

[1] GANG is the acronym of the Center for Geometry, Analysis, Numerics and Graphics.

## 2. Minimum User Requirements

**Hardware.** We request one SGI four-processor machine, one file server, plus ten $X$-terminals. The SGI will be dedicated to research projects in this proposal; the $X$-terminals would provide additional means of access to the SGI for faculty, graduate students and visiting collaborators working on these projects; the file server will handle the data traffic generated by these projects and will also support the X-terminals.

For security reasons, our current network is set up so that each faculty member has access to the workstation in his own office plus four publicly accessible workstations. These workstations are primarily Sun Ultra Sparc 2 to 5. In particular, each person has very limited CPU access, both in terms of the number of processors available and in terms of the raw computational power per processor. On the other hand, the very nature of our projects — Monte Carlo simulation, multiscale hybrid algorithm, symbolic computation, and graphics animation — require intensive CPU and memory usage. We request an SGI Origin 200 machine, with 2Gb of RAM, four 64 bit R12000 processors running *in parallel* at 270 MHz, and 4Mb of level-2 cache per processor. This allow will us to utilize graphics software developed exclusively for the SGI platform by GANG Research Group. The large L2 cache will significantly improve the speed for symbolic computation. In addition, the SGI is equipped with custom-made C and Fortran compilers which automatically parallelize computer code, allowing us to readily make full use of all four processors.

In the course of investigating the projects proposed here, we expect to bring in collaborators and to attract graduate students working on these projects. This requires additional access to the proposed SGI machine. Currently, the 70 graduate students in the Department have access to eleven computers, and only four of them are UNIX workstations. Furthermore, the Department's current file server does not have the capacity to handle the additional load generated by these projects. We thus request funding for ten NCD Explorer 401 Thin Client X-terminals plus one file server, dedicated to these projects.

**Software.** Our budget includes an access fee for 10 simultaneous sessions of Matlab. This fee varies slightly from year to year, averaging $30 to $35 per user per year. We also request a site license for Maple as an integrated environment for symbolic, numerical and graphical work.

**In summary,** the minimum user requirements for this proposal call for a four processors machine running in parallel at the 300MHz range per processor, 2Gb of RAM and large level-2 cache; a file server with 18Gb storage; ten $X$-terminals, a color laser printer, and site licenses for Maple and Matlab.

## 3. Detailed Research Projects

(i) **Computation in Algebraic Geometry** (Eduardo Cattani, David Cox, Frank Sottile)

Until recently, algebraic geometry was known chiefly for the depth and abstraction of its techniques and results. Concrete questions were often insoluble and not central to the subject. This has begun to change due to improvements in computational power coupled with theoretical advances expressed in optimized software packages, and the dissemination of these ideas through textbooks [9]. Computer experimentation is now a viable tool for mathematical discovery in algebraic geometry.

An important and practical, yet challenging problem is to find (or understand) the solutions to a system of multivariate polynomial equations

$$f_1(x_1, \ldots, x_N) \;=\; \cdots \;=\; f_n(x_1, \ldots, x_N) \;=\; 0\,. \tag{1}$$

This problem is further complicated when real-number (as opposed to complex-number) solutions are desired. This is often the case of most interest, as applications demand such real solutions. (Real) enumerative geometry is the geometric counterpart of this question. It studies questions like the following:

(2) How many lines meet four general lines in space?

More generally, enumerative geometry studies the geometric figures in a family (in this case, lines in space) that satisfy conditions imposed by general, fixed figures (meet four general lines). When the fixed figures are real, some solutions will be real, while the rest occur in complex conjugate pairs, and the distribution of these two types depends subtly on the configuration of the conditions. For example, given 4 real lines, there are either 0 or 2 real lines meeting all 4. In most known cases, all solutions *can* be real. These include the 40 positions of the Stewart platform in robotics [10], the 12 lines tangent to four spheres from computational vision [18], and the feedback laws that stabilize a linear system in systems theory [12].

The Schubert calculus of enumerative geometry, of which (2) is an example, is a fruitful class of problems to address these questions of real solutions. This studies linear subspaces of a vector space satisfying incidence conditions imposed by other (fixed) linear subspaces. These questions arise in applications, as families of linear subspaces (*Grassmannians*) are a natural compactification of spaces of matrices.

A conjecture of Boris Shapiro and Michael Shapiro has inspired recent significant progress in this area [14]. They conjecture that if the fixed linear subspaces osculate a given rational normal curve at real points, then all incident subspaces are real. This exact problem was studied in both linear systems theory and the moduli of curves, but no connection to the real numbers was observed. Significant computer experimentation [14, 19] suggests their conjecture is true. These experiments led to the advances of [12] and [13], which showed it is possible to have all solutions be real for some questions of the classical and quantum Schubert calculus on Grassmannians. They also inspired work that led to the recent advance [11], which implies Shapiros's conjecture when the subspaces have dimension 2.

The Schubert calculus also considers subspaces which are isotropic with respect to a given non degenerate bilinear form. When the form is symmetric, a relevant space is the (*maximal*) *orthogonal Grassmannian* which is a compactification of the space of skew-symmetric matrices. When the form is alternating, we have the *Lagrangian Grassmannian* which is a compactification of the space of symmetric matrices. We also consider flags of subspaces, obtaining the *flag manifold*.

Computer experimentation has shown that the obvious extension of Shapiros's conjecture (incidence conditions imposed by subspaces osculating a rational normal curve) to these other manifolds is false [14]. Yet one may still prove interesting questions of reality. For example, many such enumerative problems on the orthogonal Grassmannian can have all their solutions be real, and the same is true for the flag manifold [15]. For the Lagrangian Grassmannian, we meet a new phenomenon—many such enumerative problems can have no real solutions [15].

Limited computer experimentation indicates that Shapiros's conjecture may have some extension to these spaces. For the orthogonal Grassmannian, it appears there will be only real solutions for any choice of conditions imposed by real osculating flags. For the Lagrangian Grassmannian, these computations suggest that for a given enumerative problem, the number of real and complex solutions does not depend upon the points of osculation. However, we have been unable to predict what the numbers will be, as very few examples are feasible. The most interesting case is the flag manifold. Here, some computations suggest that if the osculation points are chosen in a particular order, then all solutions will be real, but this is very subtle. Again, not enough examples can be computed at present. (See [15] for a more thorough discussion.)

In addition to the symbolic methods used above, there are numerical homotopy techniques for these problems on the Grassmannian used to study the original conjecture of Shapiro and Shapiro [19]. There are likewise homotopy methods for these other spaces. We plan (perhaps with students or external coauthors) to implement these inherently parallelizable algorithms and use them to address these questions of reality. Lastly, the spaces mentioned here do not exhaust all flag manifolds, and we plan further experimentation to help study this important problem of reality in enumerative geometry.

Perhaps the most exciting development in algebraic geometry in the last decade has been the verification of some formulas from physics predicting the number of solutions to certain enumerative problems involving curves in various spaces. An early chapter in this story was the quantum cohomology of Grassmannians. There the numbers count rational curves on a Grassmannian that satisfy certain Schubert conditions at certain points. (This problem arose independently in control theory, where it was originally solved.) A new verification of these numbers for Grassmannians is a consequence of the form of an elegant Gröbner basis for a singular compactification of the space of curves in the Grassmannian [16]. Several stages in the search for this Gröbner basis were crucially informed by large-scale computer experimentation which was extremely challenging to execute and interpret.

It is likely that we can apply such Gröbner basis techniques to extend these results to spaces of curves in other flag manifolds (where we also expect interesting real-number phenomena). That important project will require serious computer experimentation. We also propose a more ambitious application of this symbolic approach to enumerative geometry which is suited to the interests and expertise of our group. Alexeev [1] finds a rich combinatorial structure (fibre polytopes) describing spaces of maps between toric varieties. We would like to study a common generalization of this and [16]: The enumerative geometry of maps from toric varieties to Grassmannians via spaces of maps. Preliminary experimentation shows this generalization will require non-trivial new ideas and new combinatorial structures. Serious computational experimentation will prove crucial in furthering this project.

Even partial results should give rise to an interesting new family of solved enumerative problems—counting toric subvarieties of Grassmannians that satisfy certain Schubert conditions at certain points. These new enumerative problems will pose a challenge to algebraic geometry—find a theoretical framework similar to Gromov-Witten invariants or quantum cohomology (which come from the work on curves in varieties) to solve these enumerative problems. We also expect to find some interesting reality phenomena mixing the results of [13] (where all solutions can be real) with the situation for sparse equations [17] (where not all solutions are real, but lower bounds on the number of real solutions do exist).

An important tool for studying Gromov-Witten invariants of toric varieties and their hypersurfaces is the Gelfand-Kapranov-Zelevinsky theory of hypergeometric functions. This is one of the recent research interests of Eduardo Cattani, who has studied rational hypergeometric functions in [5]. The denominators of these rational functions are conjectured to be certain resultants. These resultants also appear as denominators of toric residues [4]. The theory of toric residues is developed in [2, 3, 6].

David Cox's recent research interests involve the commutative algebra which arises in computer aided geometric design. The early work in this area used classical resultant theory, but more recently, other areas of commutative algebra, including syzygies and the sheaf cohomology, have been used [7, 8]. For example, the *implicitization* problem asks for the equation of a parametrized surface in $\mathbb{P}^3$. Standard techniques, such as Gröbnber bases, are too slow for real-time computations. Newer, more efficient algorithms use syzygies to express the equation as a determinant. This line of research combines computational methods (benchmarking and computing examples) and theoretical challenges (finding appropriate genericity conditions under which the algorithms can be proved to work).

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(ii) **Computational Number Theory** (David Hayes, Siman Wong)

From calculus we learned that

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \frac{1}{11} + \frac{1}{13} - \cdots \tag{3}$$

This is in fact a concrete instance of the *Dirichlet Class Number Formula*. For any square-free, positive integer $d$ and for any prime number $p > 2$, define the *quadratic symbol for* $-d$ to be

$$\left(\frac{-d}{p}\right) = \begin{cases} 0 & \text{if } p \text{ divides } d; \\ 1 & \text{if } p \text{ does not divide } d \text{ and if } p \text{ divides } n^2+d \text{ for some integer } n; \\ -1 & \text{if } p \text{ does not divide } d \text{ and if } p \text{ does not divide } n^2+d \text{ for any integer } n. \end{cases} \tag{4}$$

We can extend this so that $\left(\frac{-d}{n}\right)$ is defined for all positive integers $n$. The Dirichlet Class Number Formula then says that the series $\sum_{n=1}^{\infty}\left(\frac{-d}{n}\right)\frac{1}{n}$ converges (conditionally) to $\pi/\sqrt{d}$ times an explicit fraction whose numerator is intimately related to a crucial arithmetic invariant of the quadratic field $\mathbb{Q}(\sqrt{-d})$, called the class number of the quadratic field. For $d = 1$ the Formula specializes to (3), which expresses in analytic terms the well-known fact that the ring of Gaussian integers $\mathbb{Z}[\sqrt{-1}]$ is a unique factorization domain.

The series $\sum_{n=1}^{\infty}\left(\frac{-d}{n}\right)\frac{1}{n}$ is none other than the value at $s = 1$ of the function $L(s, -d) := \sum_{n=1}^{\infty}\left(\frac{-d}{n}\right)n^{-s}$. It turns out that $L(s, -d)$ is the Mellin transform of a modified theta function and admits a functional equation relating $L(s, -d)$ to $L(1 - s, -d)$. Furthermore, the celebrated Quadratic Reciprocity Law of Gauss shows that $\left(\frac{-d}{p}\right)$ is determined by the congruence class of $p$ modulo $4d$, thus allowing us to rapidly compute the terms of $L(s, -d)$.

To say that $p$ divides $n^2 + d$ is equivalent to saying that the polynomial $x^2 + d$ has a root modulo $p$. Given a polynomial $f(x)$ over $\mathbb{Q}$, we can then ask if there is an '$f$-symbol' $\left[\frac{f}{p}\right]$ analogous to (4), whose value at a prime $p$ is related to the factorization of $f(x)$ modulo $p$. And if such symbols make sense, is the generating function $L(s, f) := \sum_{n=1}^{\infty}\left[\frac{f}{n}\right]n^{-s}$ equal to the Mellin transform of a well-behaved analytic function? Do values of $L(s, f)$ at special values (e.g. $s = 0$) encode arithmetic information about $f$?

One can indeed make precise the notion of a '$f$-symbol'. This turns out to be closely related to irreducible representations of the Galois group of $f$, and the corresponding $L$-function is called an Artin $L$-function. The Langlands program predicts that these Artin $L$-functions are Mellin transforms of a very special type of complex analytic functions called automorphic forms. In the case where $f$ is a cyclotomic polynomial, this vast program encompasses as a special case a famous theorem of Dirichlet, which says that every arithmetic progression contains infinitely many primes if the first two terms have no common factor.

In many arithmetic problems, we start with automorphic forms and we try to deduce from them number theoretic information. For instance, questions about class numbers of cubic fields readily lead to automorphic forms corresponding to quartic polynomials whose Galois groups are the symmetric group or the alternating group on four letters [9]. To extract arithmetic information from these special automorphic forms we then need to separate them from those corresponding to quartic polynomials with dihedral Galois groups. In Wong's project we propose to distinguish automorphic forms of different Galois type based on the distribution of the values of these forms as complex analytic functions. Equally important in the arithmetic study of automorphic forms are the coefficients of their Mellin transforms. In a series of papers, Stark formulates conjectures which predict that the leading terms of Artin $L$-series generate specific Abelian extensions of number fields (see [6], [7]) . Due to the difficulties in computing these $L$-series, until recently the Stark conjectures have been verified for a very limited number of non-Abelian cases. In Hayes' project we propose to implement a polynomial-time algorithm to compute these $L$-series. The data collected will help better understand the Stark conjectures, and possibly lead to a new integer factorization algorithm.

### Computing Brumer elements over totally real Number Fields

Let $k$ be a number field, let $S$ be a finite set of places of $k$ containing at least all the archimedean places of $k$, and let $k_S$ be the maximal abelian extension of $k$ that is ramified only over the places in $S$. If $K/k$ is a finite sub-extension of $k_S/k$, then class field theory provides an algorithm which uses input information in the base field $k$ to solve arithmetic problems in the over field $K$. The input information is the conductor ideal $\mathfrak{f}_K$ of $K/k$ together with a finite set of ideals $I_K$ of $k$ that generate $\mathrm{Gal}(K/k)$ under the Artin map. Unfortunately, the theorems of class field theory are proved indirectly and so they do not imply efficient algorithms for computation in $K/k$.

Although currently open, the Stark conjectures (see [6] and [7]) do provide efficient algorithms for arithmetic computations in $K/k$ from the input information $\mathfrak{f}_K$ and $I_K$. The conjectures assert that the lead terms in the Taylor expansions of the complex partial zeta-functions $\zeta_S(s, \mathfrak{a})$ associated to the ideals $\mathfrak{a} \in I_K$ at $s = 0$ contain specific information about canonical elements in $K$. This information is most easily available in the case when at least one of the zeta-functions has a first order zero at $s = 0$. Since these zeta-functions are defined by the arithmetic of $k$, they are computable when $k$ is computable.

The Stark algorithm requires the insertion of a split place $v$ into $S$ and uses the resulting embedding of $K$ into the completion of $k$ at $v$. When $v$ is archimedean, the conjectures have been successfully implemented in the PARI software package. This implementation is an order of magnitude more efficient then other currently available algorithms. Even though the conjectures are not proved, when the algorithm produces a result, it is easy to verify independently that the result is correct.

The algorithm required when the split place $v$ is non-archimedean is quite different from the archimedean one. When $k$ is a real quadratic number field, the non-archimedean algorithm is the continued fraction algorithm (see [3]). Recently, Gunnells and Szcech [2] have found a polynomial time algorithm for computing the partial zeta-values at $s = 0$ over *any* totally real number field $k$. When $v$ is non-archimedean, the relevant partial zeta-values are rational integers which therefore may be computed with infinite precision. Also, these values may be computed without computing a data base of norms, which is the most time consuming part of the archimedean algorithm. It is reasonable to hope therefore that the use of the Gunnells-Szcech algorithm will provide a substantial improvement in efficiency.

Hayes is currently working with Gunnells and Szcech to implement their algorithm on a computer. Apart from the application to computations in number fields, another possible application is to the problem of factorization of large integers. This possibility arises from the observation (see [3]) that the denominator of the rational values $\zeta_S(s, \mathfrak{a})$ are often smaller than the maximum predicted by the theory. In other words, the predicted value is factored. If one could establish firm estimates for the frequency with which this phenomenon occurs, it might lead to a new factoring algorithm.

## How to color an automorphic form

Let $k/\mathbb{Q}$ be a quartic field whose Galois group is the symmetric group $S_4$ or the alternating group $A_4$. Both of these groups can be viewed as subgroups of $PGL_2(\mathbb{C})$, so the Galois closure of $k/\mathbb{Q}$ can be viewed as the splitting field of an irreducible *projective* representation $\tilde{\rho} : Gal(\overline{\mathbb{Q}}/\mathbb{Q}) \to PGL_2(\mathbb{C})$. Tate shows that such $\tilde{\rho}$ can be lifted to an ordinary representation $\rho : Gal(\overline{\mathbb{Q}}/\mathbb{Q}) \to GL_2(\mathbb{C})$. By the work of Langlands-Tunnells ([5], [8]), the Artin $L$-series associated to $\rho$ is the Mellin transform of an automorphic form on $GL(2)$. But quartic polynomials with dihedral Galois groups also give rise to such automorphic forms, and as explained in the opening paragraphs, it is of great number theoretical importance to separate these two types of forms.

Consider the case where the automorphic form comes from a representation $\rho$ where the order of $\det \rho$ is fixed. Then the image of this representation has fixed order. In particular, as $p$ runs through all prime numbers, the $p$-th Fourier coefficients of the automorphic form can take on only only finitely many values. Moreover, the Chebotarev density theorem prescribes the distribution of these values depending on whether or not the representation is dihedral. Since the distribution of the Fourier coefficients of the automorphic form depends on the Galois type of the representation, this suggests that the distribution of these values of the automorphic form, viewed as an complex analytic function, will be influenced by the Galois type as well. In order to test these heuristics we need to generate non-dihedral forms and to plot the values of these complex analytic functions.

To visualize a complex-valued function in the plane we use what Farris [1] called domain coloring diagrams. This is similar to the color-by-Gauss map method used by differential geometers to visualize surfaces in space. We begin by coloring the complex plane as one does in a traditional color wheel: Put red at the complex number 1, with green and blue at the other two cube roots of unity. Hues are interpolated, giving secondary and tertiary colors. Blend toward white at the center, toward black going outwards. Thus, each complex number has a color associated to it. Given a complex-valued function $f$, for each pixel in the domain of $f$ we then compute the color associated with that input value and use that color for that pixel.

We now focus our attention to color automorphic forms. We have developed an algorithm to generate non-dihedral forms of bounded conductors. This makes use of symbolic computations in class field theory, searches of tables of cubic and quartic fields, and computing about 1000 terms of each of the non-dihedral automorphic forms. This requires extensive resources in both symbolic computations and fast integer arithmetic, in addition to large storage. In addition to the study of Artin $L$-series, these data will be useful in constructing weight 3/2-modular forms which are congruent to Artin $L$-series, a device useful for constructing elliptic curves with non-trivial Tate-Shafarevich groups [10]. Finally, given an (non-dihedral) automorphic form $f$, we need to compute a connected fundamental region for $f$ and then plot the domain coloring diagram over this domain. This requires evaluating (using floating-point arithmetic) the 1000-term power series obtained above at hundreds of points of the fundamental region, and then output the corresponding color. This time-consuming computation can be sped up significantly if it can be performed on a parallel machine with large memory.

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**(iii) Mesoscopic Theories and Hybrid Computational Algorithms in Materials Science and Fluid Mechanics** (David Horntrop, Markos Katsoulakis, Bruce Turkington)

Many important physical phenomena involve a large number of interrelating spatial and temporal scales. The modeling and computational challenges of these problems are formidable due to their inherent non-linear nature and the disparity of active scales. Stochastic models, derived for instance from statistical mechanics, play a crucial role in describing such phenomena at a microscopic level, while on the other hand phenomenological, continuum models are employed at macroscopic scales. Our project proposes to develop suitable mesoscopic models at intermediate scales which, while incorporating microscopic information, have many of the attractive computational and analytical features of the macroscopic, PDE-based models. The two main examples we propose to explore here are mesoscopic theories for (i) catalytic reactors and material synthesis, and (ii) two-dimensional freely decaying turbulence.

Mesoscopic theories for catalytic reactors and materials synthesis

Modeling and simulation of physicochemical phenomena over multiple, interconnected length and time scales poses one of the most challenging mathematical and computational problems for the science and engineering communities. Critical steps in this effort are, (a) the integration of quantum mechanics results in molecular and continuum models, and of molecular (microscopic) in continuum (macroscopic) models, as well as (b) the development of suitable hybrid algorithms for coupled multiple scales that interweave Monte Carlo or molecular dynamics, with continuum models.

In [1, 2] we study cluster formation and propagation in catalytic reactors, although the techniques developed may apply to a wide spectrum of advanced materials synthesis such as deposition processes and thin films. The prototypical physical model we studied in [1] consists of the molecular adsorption of species $A$ from a gas phase (reactor) onto a catalytic surface. The adsorbed species $A^*$ can either desorb back into the fluid phase, diffuse on the surface, or react through a unimolecular surface reaction to give product $B$. The surface processes (adsorption, desorption, surface diffusion, etc.) lead to the formation of clusters that evolve undergoing topological changes and simultaneously interacting with the gas phase. The models that have been developed to date mainly address distinct length and time scales. On one hand, Monte Carlo algorithms describe the surface processes at the molecular, microscopic level. At the other extreme, continuum fluids equations describe the flow, transport, and chemistry in the gas phase and are suitable mostly for long scales.

One of our primary goals is to develop a general mathematical and computational framework for linking such multiple length and time scales phenomena. One of the important mathematical tools here is a mesoscopic theory for the surface processes, derived from the microscopic models, by means of a *local* mean field approximation, (see also [3-5] and references therein for related derivations in non-equilibrium statistical mechanics). The average coverage $u$ of the surface solves [6,1]:

$$u_t - D\nabla \cdot \Big[\nabla u - \beta u(1-u)\nabla J_m * u\Big] - \Big[k_a p(1-u) - k_d u \exp\big(-\beta J_d * u\big)\Big] + \xi(x,t) = 0\,. \tag{5}$$

Here $J_d$ and $J_m$ are the intermolecular potentials for surface desorption and diffusion and $\xi = \xi(x,t)$ is a space/time random perturbation describing microscopic fluctuations of the system. Furthermore, $D$ is the diffusion constant, $k_d$, $k_a$ denote respectively the desorption, and adsorption constants, $p$ is the partial pressure of the gaseous species $A$, and $J * u$ denotes the convolution. Related models where only the diffusion mechanism is present describe kinetics of phase separation in polymer mixtures (see [7] and references therein).

Mesoscopic theories such as (5) allow us to drastically simplify the coupling of the surface processes with the macroscopic equations in the gas phase, but simultaneously include microscopic information moving beyond a simple phenomenological description [2]. Furthermore this theory yields macroscopic laws for the formation, propagation and interaction with the gas phase of surface clusters [1].

The computational challenges we face here are two-fold: We first need to develop efficient Monte Carlo/deterministic techniques for mesoscopic equations such as (5), and secondly combine the resulting algorithm with a numerical scheme for the continuum gas phase in a single hybrid algorithm that is partly Monte Carlo and partly deterministic. To complete the first task, we plan to develop an efficient spectral algorithm for the simulation of the deterministic version of (5), possibly using wavelet decompositions based on the intermolecular potentials at hand [8]. Next we intend to develop suitable techniques that incorporate the random fluctuations of (5) and compare them to benchmark microscopic calculations for the underlying particle systems. Note that the random fluctuations here are critical in triggering surface phenomena through spinodal decomposition and nucleation.

Mesoscopic theories for two-dimensional turbulence

Another important area which we plan to study computationally through the use of mesoscopic models is freely decaying two-dimensional turbulence. While certainly very physically different than three-dimensional turbulence, two-dimensional turbulence is still physically relevant and is observed in many geophysical flows in the atmosphere and ocean ([9],[10]) as well as in astrophysical flows ([11]). Such situations are characterized by the appearance of large scale coherent vortices surrounded by a sea of small structures. An inviscid, two-dimensional, ideal flow is described by the Euler equation

$$\frac{\partial \omega}{\partial t} + v \cdot \nabla \omega = 0 \tag{6}$$

where $v$ is the velocity field and $\omega = \nabla \times v$ is the vorticity field. The condition $\nabla \cdot v = 0$ is needed to enforce incompressibility of the flow.

This nonlinear problem (6) has proved to be very difficult to tackle for a wide variety of reasons. While it has been proven that smooth solutions of (6) exist at all times given smooth initial data ([12]), in practice the solutions rapidly develop very filamentary structure. Thus, this problem is quite difficult to solve numerically to a high degree of accuracy through a standard discretization of the partial differential equation due to the large number of scales that naturally arise.

Rather than attempt such a deterministic approach for a computational study of two dimensional freely decaying turbulence, we plan to use simulation based on a statistical mechanics framework. The use of statistical mechanics to describe turbulent velocity fields was pioneered by Onsager in 1949 ([13]) with many improvements and generalizations continuing to the present ([14],[15],[16]). Basically, a valid statistical mechanics description of a velocity field should have readily observable coherent structures in the most probable equilibrium state. This state is determined by maximizing the entropy of the system while preserving the values of conserved quantities such as energy and entropy. This approach yields in a suitable limit a mesoscopic theory for equilibrium two-dimensional turbulence. The resulting optimization problem can be solved in an efficient manner using the algorithm recently developed by Turkington and Whitaker ([17]).

The goal of this project is to develop a nonequilibrium statistical mechanics theory that will describe freely decaying two-dimensional turbulence. In other words, we wish to gain insight as to how the coherent vortices organize, grow, and merge as time progresses to eventually form the large vortices amid a sea of small swirls so commonly observed in nature. As a first step in the development of this theory, we assume that the system is in quasi-equilibrium. Such an assumption means that the underlying mechanism determining the state of the system (the prior distribution) takes a much longer time to evolve than is required for the system to equilibrate. Thus, it is possible to use equilibrium statistical mechanics theories at each time step to determine the most probable vortex configuration. Certainly, the validity of the quasi-equilibrium assumption is crucial in this study and will be checked through a comparison with direct numerical simulations of (5). Another important feature of our proposed statistical mechanics theory is that at a given time it must be possible to find multiple vortex configurations with the same entropy and conserved quantities since realistic fluid flows have many configurations with the same physical properties. While this task could prove to be quite computationally intensive, our preliminary results ([18]) indicate that it is indeed possible to find such families of physically equivalent vortex configurations. Given the validity of these assumptions, we should then have a much faster and more accurate means of calculating two-dimensional freely decaying turbulence thereby being well on the way to having a nonequilibrium theory which will enhance our understanding of these physically important flows.

## Conclusion

The problems described in the two preceding sections are of fundamental interest in the science and engineering communities, as well as in industry. Thus far these problems have proven to not be easily amenable to traditional computational techniques. Here we proposed the development of new mesoscopic models and their accompanying hybrid computational algorithms, combining Monte Carlo and deterministic numerical methods. Our group of researchers brings to bear a unique blend of expertise in equilibrium and non-equilibrium statistical mechanics, nonlinear PDE, and stochastic and deterministic numerical methods. Furthermore the proposed project builds on already existing collaborations among the three co-PIs and their Ph.D. students.

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## (iv) **Geometry, Computation and Visualization** (Robert Kusner, Nicholas Schmitt)

### CMC surfaces and loop groups

Constant mean curvature (CMC) surfaces, which are equilibrium surfaces of area variation with a volume constraint, model fluid droplets under surface tension, and are also of intrinsic geometric interest. One of the challenges over the past century has been to find an effective way to explicitly compute complete CMC surfaces.

Unlike their zero mean curvature counterparts, the minimal surfaces, which can be computed using the meromorphic Weierstrass representation, CMC surfaces have until recently been understood primarily via PDE methods. The finest examples of this analytic approach include Wente's resolution of the Hopf Conjecture [14] and the fusing constructions of Kapouleas [6, 7, 8]. More recently a meromorphic approach to construct CMC surfaces has been described in a paper [2] by Dorfmeister, Pedit and Wu (DPW) using the loop group formulation of harmonic maps.

Our research focuses on the construction and classification of new families of CMC surfaces by means of the DPW theory. `DPWLab`, a software package developed at the GANG Research Group by Nicholas

Schmitt, implements this theory and has been extremely effective for interactively computing, visualizing and investigating new and known CMC surfaces.

Investigations with `DPWLab` has lead us to understand how to read geometric information about a CMC surface from its DPW input data. For example, simple poles in the DPW meromorphic potential lead to Delaunay ends, and higher order poles to 'Mr. Bubble'- (or Smyth surface-) type ends. The fusion of various end types can be effected by linear superposition on the level of meromorphic potentials. We have used this method to fuse Delaunay and Mr Bubble type ends to obtain new CMC cylinders [10].

Of primary importance is the holonomy or period closing problem, that is, simultaneously closing the CMC surface at each of its ends. The DPW approach to this problem involves the linear superposition paradigm. To construct $n$-oids with Delaunay ends, one constructs meromorphic DPW data with $n$ simple poles on a compact Riemann surface. The free parameters involved in the potentials relate to the end weights and are discussed by Kusner et. al. [3, 4]. Indeed, the experimental output from `DPWLab` is in complete agreement with the known CMC moduli space theory [11, 5]. We propose to use this new way of thinking about these parameters as an approach to investigate the detailed structure of the unknown moduli spaces.

Controlling the holonomy requires a careful analysis of a Riemann-Hilbert problem. It is classically known that for a Riemann sphere with three punctures the holonomy can be parametrized by hypergeometric functions. Preliminary results from `DPWLab` indicate that this construction can be carried out and will describe the moduli of trinoids of Delaunay end type (nodoidal and unduloidal) in terms of the residues of the meromorphic connection [13].

We propose to apply these methods to the case of more then three ends. Even though the Riemann-Hilbert problem can no longer be solved explicitly for this case, one still expects to be able to prove existence for the various Delaunay type end configurations and describe their moduli. We also propose to adapt these software tools to the study of Willmore surfaces, which are equilibria for the $L^2$-norm of the mean curvature; this energy models the elastic bending energy of certain membranes. From the loop group viewpoint Willmore surfaces in 3-space and 4-space can be viewed as quaternionic analogues of CMC surfaces. The resulting factorization and holonomy problems are computationally much more intensive and will heavily utilize parallelized software on the new multiprocessor SGI machine.

#### The `DPWLab` implementation

`DPWLab` is the premier software for interactively constructing, visualizing and investigating CMC surfaces. `DPWLab` has been effective for understanding known surfaces and creating new examples, including tori, bubbletons, generalized Smyth Surfaces, and cylinders with umbilics. `DPWLab` was crucial in the discovery of new constant mean curvature examples, including cylinders with Smyth and Delaunay-type ends, and immersed $n$-oids. The heart of `DPWLab` is a collection of highly optimized algorithms to perform loop group factorizations via QR and Cholesky matrix decomposition.

The DPW procedure involves several computational steps:

- solving numerically a first-order initial value problem with variable in the appropriate loop group;
- applying the Iwasawa decomposition to this solution pointwise to obtain the extended Gauss map for the CMC surface;
- computing the the CMC surface from its extended Gauss map using the Sym-Bobenko formula;
- computing appropriate initial condition to close holonomy.

The differential equation of the first step is solved by fourth-order Runge-Kutta methods. Since the loop algebra elements in question are, from the numerical point of view, a matrix whose entries are Laurent series expansions, the `DPWLab` implementation performs its computations with finite vectors representing truncated Laurent expansions with user-definable length.

The Iwasawa decomposition, the heart of the DPW procedure, has been implemented and optimized for the first time in `DPWLab`. This step, the most time-consuming and numerically unstable part of the DPW computation, is reducible to the problem of computing, at each meshpoint of the CMC surface to be generated, projections to linear subspaces generated by loop group elements. `DPWLab` offers the user a choice of methods, Cholesky decomposition and QR-decomposition, to optimize this part of the calculation.

Once this factorization is performed, the full geometric data — metric, Gauss map, and Hopf form — for the CMC surface and its associate family are computed.

CMC surfaces whose underlying domain has topology require initial conditions (dressing matrix) which close the surface; these are found by numerically minimizing the normal and translational periods on the surface using conjugate gradient methods. Using these tools, we have computed families of embedded CMC trinoids and trinoids with nodoid ends, as well discrete families of $n$-oids with coplanar and non-coplanar end configurations. We propose now to investigate the entire moduli spaces of non-coplanar CMC surfaces using these methods.

Computational aspects of `DPWLab`

`DPWLab` is a package tuned to the SGI/IRIX hardware/OS configuration. Because of its two-pronged computational and visual elements, `DPWLab` has a demanding hardware footprint.

The interactive facet of `DPWLab`'s visual/graphical component allows the user to display, move, cut away, flow through, and deform CMC surfaces in real time. It also has automated video production facilities, with which the user can record single surfaces in motion or generate animations of CMC families. This graphics component performs optimally with the OpenGL API and the high-performance graphics capability of Silicon Graphics machines.

This visual/graphical aspect of `DPWLab` is secondary to its primary task of computing triangulated CMC surfaces in 3-space. Adjunct to the `DPWLab` package proper is an array of holonomy or period-closing tools which typically use conjugate gradient methods to minimize functionals on infinite-dimensional loop algebras, appropriately truncated. For CMC surface computation, `DPWLab` is fully multithreaded to take advantage of multiprocessor machines.

Our primary test bed for `DPWLab` is two Silicon Graphics Octane workstations with dual R12000/R10000 processors. The package runs optimally with at least 512 megabytes of main memory. Hard disk storage requirements can be heavy, especially when creating, rendering and storing video sequences. The new multiprocessor SGI will help make the real-time investigation of moduli spaces of surfaces possible.

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## 4. Plan for maintenance & Operations

The Mathematics and Statistics Department is networked for computer access to the local ethernet connection. The University will allocate the space for a computer lab and pay for the costs of any renovation that may be necessary. The SGI machine and the file server will be housed in an existing machine room. The X-terminals will be housed in the computer lab except that several will be installed in the two existing computer rooms for public access by graduate students involved with these projects. The faculty can access the SGI and the file server from workstations in their offices.

The Department will employ a full-time professional System Administrator to set-up this equipment in the new computer lab, and to oversee daily operation. We request 50% salary plus fringe benefits for this position for two years. The University will assume the full personnel costs after NSF funding ends. The System Administrator will be assisted by two graduate student computer coordinators, on tasks such as routine hardware maintenance and certain software support. These two graduate students have no departmental duties other than those toward the system, and the Department provides full graduate student stipend plus fringe benefits for their work ($17780 per year per graduate student — one dedicated to this project).

## 5. Currently Available Equipment

The present computing facilities of the Mathematics and Statistics Department consists of the following equipment:

| Qty | Item | Age |
|---|---|---|
| 2 | SGI Octane R10000 | 6 & 18 months, resp. |
| 2 | SGI Indigo2 R10000 | 3 to 4 years |
| 1 | SGI Indigo R4000 | 4 years |
| 1 | SUN Sparcserver 10 model 52, running SOLARIS 2.5, with 96M RAM and 9G storage (Departmental file server) | over 10 years |
| 4 | Sun Ultra 5 and 10 Workstations (for public access) | 18 months |
| 7 | Assorted PC and Macintosh (for public access) | 1 to 4 years |

In addition to this equipment, there is one workstation in every faculty member's office (primarily Sun Ultra 2 and Ultra 5 workstations, purchased during the last 1 to 5 years). As we explained in the section 'Minimal User Requirements', our network is setup so that every faculty has access to the workstation in his office only plus the four public Sun Ultra workstations. These four Ultra workstations plus the seven PC and Mac are used primarily by the 70 graduate students in the Department for word processing and other course work. This equipment, along with the workstations in faculty offices, is currently maintained by one full-time system administrator along with three assistants.

**Biographical Sketch**

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**Recent Significant Publications:**

- On the density of elliptic curves. To appear in *Compositio Math.* (34pp)
- Automorphic forms on $GL(2)$ and the rank of class groups. *J.Reine Angew. Math.* **515** (1999) 125-153
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- Twists of Galois representations and projective automorphisms. *J. Number Theory.* **74** (1999) 1-18

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- (with A. Majda) An overview of Monte Carlo simulation techniques for the generation of random fields, in: *Monte Carlo Simulations in Oceanography, Proc. Ninth 'Aha Huliko'a Hawaiian Winter Workshop* 1997, p. 67-79.
- (with F. Elliott and A. Majda) A Fourier-wavelet Monte Carlo method for fractal random fields. *J. Comp. Phys.* **132** (1997) 384–408.
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- (with D. G. Vlachos) ¿From microscopic interactions to macroscopic laws of cluster growth. To appear in *Phys. Rev. Lett.*
- (with S. Jin and Z. Xin) Relaxation Schemes for Curvature-Dependent Front Propagation. *Comm. Pure Appl. Math.* **52** (1999) 1587–1615.
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- (with P. E. Souganidis) Generalized motion by mean curvature as a macroscopic limit of stochastic Ising models with long range interactions and Glauber dynamics. *Comm. Math. Phys.* **169** (1995) 61-97

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- (with K. G. Brauckmann and J. Sullivan) Constant mean curvature surfaces with three ends. To appear in *Proc. Nat. Acad. Sci.* (*USA*)
- (with K. G. Braukmann) Embedded constant mean curvature surfaces with special symmetry. *Man. Math.* **99** (1999) 135-150
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- (with Nantel Bergeron) Schubert polynomials, the Bruhat order, and the geometry of flag manifolds. *Duke Math. J.* **94** (1998) 273–423.
- (with B. Sturmfels) A sagbi basis for the quantum Grassmannian. To appear in *J. Pure & App. Alg.* (17pp)
- Real Schubert calculus: Polynomial systems and a conjecture of Shapiro and Shapiro. *Exper. Math.*, to appear (28pp)
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- (with B. Huber and B. Sturmfels) Numerical Schubert calculus. *J. Symb. Comp.* **26** (1998) 767–788.

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- (with D. Cox and A. Dickenstein) Residues in toric varieties. *Compositio Math.* **108** (1997) 35–76.
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- *Using Algebraic Geometry.* Graduate Texts in Mathematics. Springer-Verlag, 1998.
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- Checking the $p$-adic Stark conjecture when $p$ is archimedean. *Lec. Notes in Comp. Sci.* 1122 (1996) 91-97
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**Bruce Turkington**

**Recent Academic Employment:**

University of Massachusetts, Amherst: Associate Professor 1984-1990; Professor 1990–present

**Education:**

Stanford University. M. S., 1976; Ph. D., 1978. Thesis advisor: Robert Finn

**Recent Significant Publications:**

- Statistical equilibrium measures and coherent states in two-dimensional turbulence. *Comm. Pure Appl. Math.* **52** 781 (1999).
- (with R. Jordan) Ideal magnetofluid turbulence in two dimensions. *J. Stat. Phys.* **87** (1997) 661-695.
- (with N. Whitaker) Statistical equilibrium computations of coherent structures in a turbulent shear layer. *SIAM J. Sci. Comput.* **17** (1996) 1414–1433.
- (with N. Whitaker) Max. entropy states for rotating vortex patches. *Phys. Fluids* **A6** (1994) 3963–3973.
- (with A. Eydeland and J. Spruck) Multiconstrained variational problems in magnetohypdodynamics: equilibrium and slow evolution. *Math. Comput.* **55** (1990) 509–535.

**Coauthors** (last 48 months): Alexander Lifschitz J. Thomas Beale, Nathaniel Whitaker, Richard Jordan, Andrew Majda, Mark DiBattista, Richard Ellis, Christopher Boucher