THE DYNAMICS OF LOCALIZED COHERENT STRUCTURES AND THE ROLE OF ADAPTIVE SOFTWARE IN MULTISCALE MODELING

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Abstract. Localized coherent structures are commonplace in nonequilibrium systems, and their dynamics often dominate the response of such systems. The numerical resolution of such structures can be essential for an accurate representation of both quantitative and qualitative features of driven systems, and adaptive mesh refinement methods can play an important role in that process. But adaptivity in software must be broadly implemented beyond support just for adaptive numerical methods. Interactive problem-solving environments which support rapid prototyping, flexible exploration of numerical algorithms and strategies, extraction of salient features, and development of novel multiscale models are needed to enable real breakthroughs in the understanding of complex dynamical systems.

Key words. Localized coherent structures, dynamics of defects, problem-solving environments, adaptive software environments.

1. Introduction. Extended, nonlinear systems driven out of equilibrium often yield or fail through the formation, interaction and evolution of localized coherent structures. [1] In many material systems, for example, these localized defects – such as cracks, dislocations, or voids – can dominate the response of the system to an imposed load. In other systems, complex spatiotemporal dynamics can result when defects form in otherwise regular patterns. [2] Furthermore, it is often the *collective* dynamical behavior of many interacting coherent structures that are responsible for observed phenomena. In some cases, understanding the large-scale qualitative features of a system's evolution can depend crucially on an accurate representation of coherent structures at small length scales. [3] In many driven, extended, nonlinear systems, structure exists on many length and time scales, and realistic models must support both the description of multiscale structure and the transformation of information across length scales. For these reasons, efficient and adaptive numerical methods will continue to play an important role in simulations of the dynamics of localized structures and multiscale phenomena.

Numerical methods for structured adaptive mesh refinement (SAMR) are themselves rather complicated, however, and difficult to generalize across problem domains. These techniques have been applied the most extensively in the fields of computational fluid dynamics and computational astrophysics, most notably to the resolution of shocks in fluid flows

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and of inhomogeneous clustering in gravitational problems. We are beginning to see the development of reasonably general software environments to support pieces of SAMR methods, largely due to the use of object-oriented programming techniques which can be leveraged to create flexible, hierarchical data structures that support structured adaptive meshes and adaptively resolved fields. But the widespread utility of software for SAMR will require considerable further work in both software engineering and numerical algorithm development.

The development of adaptive data structures and numerical methods for SAMR, however, represents only one piece of a much larger software puzzle. In order for adaptive mesh methods to be useful and broadly implemented by a wide range of users, adaptivity must pervade all aspects of the software infrastructure, allowing for the extraction of localized features from large PDE-based data sets, the development of new algorithms, rapid prototyping and interpretation of models and methods, and steering and control of AMR by users where appropriate.

The body of this paper consists of two main sections. Section 2 comprises a discussion of coherent structures and their dynamics as they arise in a number of different systems. Section 3 discusses issues in the development of software for such problems, aimed at the creation of problem-solving environments for the study of coherent structures and the development of multiscale models which incorporate those structures.

2. Coherent structures in materials, fluids, geophysics and related systems. The formation of localized, coherent structures in driven, nonlinear, spatially-extended systems is commonplace across a variety of disciplines, including materials science, fluid dynamics, geophysics, neurobiology and cardiology. There is currently considerable interest in understanding the characteristic features of such structures and the universality of phenomena across problem domains. Coherent structures are not merely passive objects, however; in many cases, they are believed to control the dynamics of driven systems. Furthermore, because such structures often arise in very large and complex systems of many interacting degrees of freedom, it can be difficult to extract the essential features of such systems. One is often compelled, therefore, to develop simpler, reduced-order models which focus primarily on the coherent structures themselves rather than the background in which they arise. This sort of multiscale modeling, involving the extraction of salient features and their dynamical properties to form simpler dynamical models, can enable dramatic breakthroughs in simulation capability and scientific understanding that advances in brute force computer power are incapable of providing.

In this section, I will describe a few examples of such phenomena – both from my own work and from that of others – and describe important issues, both scientific and computational, associated with the dynamics of coherent structures and the construction of multiscale models.

2.1. Crack propagation. The formation and propagation of cracks in materials is a subject of considerable practical importance as well as fundamental theoretical interest. In elastic systems, external loads concentrate elastic stress near a pre-existing crack tip, such that the (linear) elastic stress grows near a crack tip in a manner proportional to the inverse square root of the distance from the tip. Therefore, in an elastic material with an embedded crack, the local stress shows a dominant variation near the crack tip, which produces strong deformations in a localized region. These deformations must be resolved appropriately, either through adaptive refinement methods in a continuum elastic formulation of fracture, or through more exact small-scale descriptions of the material.

Because of the potentially complex geometries of propagating crack fronts, state-of-the-art simulation of crack propagation has tended to exploit unstructured mesh methods rather than the structured methods of interest here. [4] Furthermore, because crack propagation involves the evolution of geometry and topology, it has been recognized that considerable topological information must be incorporated into the description of finite element and boundary elements meshes for use in fracture mechanics. [5] Many of the issues facing the SAMR community, such as how to remesh efficiently in the face of evolving structure, are also being addressed within the unstructured mesh community insofar as computational fracture mechanics is concerned.

Continuum elastic models of fracture mechanics must make assumptions or approximations about the constitutive behavior of materials, and there is still much to be understood concerning the fundamental physics of crack formation and propagation. Large-scale parallel supercomputers have enabled in recent years the simulation of crack propagation at an atomistic scale, revealing new information about dynamic instabilities in propagating crack tips, dislocation formation and motion, and void migration and coalescence.

Figure 1 shows a series of snapshots of such a simulation, from work by Farid Abraham, using the IBM SP at the Cornell Theory Center. [6] An initial crack is shown in the upper left; under loading, this crack front begins to nucleate a cloud of dislocation lines which propagate outward, as the crack itself begins to propagate upward through the material. Such a cloud can assist in shielding the crack tip such that propagation can be inhibited or arrested. Thus, understanding the propagation of the crack requires understanding both of the dislocation cloud, and how it interacts with the crack tip. Large-scale molecular dynamics simulations are able to represent complex interactions between coherent structures such as these, but such methods are extremely inefficient, as the vast majority of atoms respond rather benignly according to the laws of linear elasticity. Capturing such complex interactions within a simplified, reduced-order model, however, is extremely challenging.

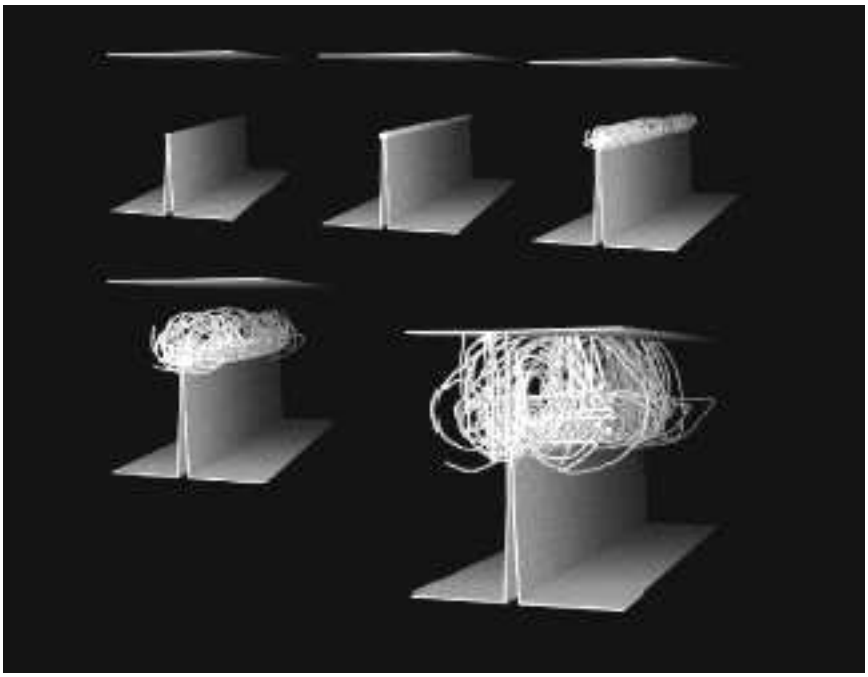

FIG. 1. *Series of snapshots of a three-dimensional atomistic simulation of fracture, by F. Abraham. External stresses are concentrated near the crack tip. In this model material, which is relatively ductile, a cloud of dislocation lines is emitted from the crack tip.*

2.2. Slip on earthquake faults. Closely related to the problem of crack propagation in materials is that of earthquake dynamics. The detailed dynamics of earthquakes, involving the nucleation and propagation of zones of slip along earthquake faults, is still not particularly well-understood. There has recently been considerable research on a number of dynamical models of earthquake faults aimed at understanding these "source" mechanisms, and the relationships between features of particular models, the nature of propagating slip modes, and the long-time statistical nature of earthquakes on driven fault systems. [3][7][8][9][10][11] A characteristic feature of many of these models – arising from the weakening character of the frictional interaction on the fault and the inertial nature of the underlying elastodynamics – is the formation of relatively sharp and localized pulses of slip that propagate along the fault away from an earthquake's epicenter.

Investigations by Heaton[12] on the "dislocation rise times" of several large earthquakes suggest that such events evolve through the propagation of "self-healing pulses of slip", whereby only localized patches of the fault are engaged in active slip at any given time. This scenario is in marked

contrast to many of the source models used within the seismological community, which assume a more delocalized form of deformation which persists throughout an entire earthquake. But self-healing modes such as those described by Heaton arise naturally in dynamical fault models which combine inertial dynamics with some form of weakening friction on the fault (be it slip weakening, velocity weakening, or some combination of the two through rate and state dependent frictional laws).

A snapshot of a self-healing slip mode is shown in figure 2, arising in the two-dimensional crustal plane model described by Myers, Shaw and Langer in [11]. This figure shows a pair of propagating slip pulses emanating from an epicenter (roughly halfway between the two slip pulses), shortly after the earthquake was triggered. The friction acting on the fault line (the back edge of the simulation domain) is slip weakening with a resticking, such that sharp pulses of slip form and propagate, but restick behind them along the fault. In their wake, the slip pulses also radiate into the adjoining elastic medium, producing strong shaking in the earth. The details of this propagation – the shape of these slip pulses, how fast they propagate, how they start and stop – are all intimately connected to dynamics on small length scales, which are governed by the nonlinear friction. [3][9] Inadequate resolution of those small scales in computational models can lead not only to quantitative inaccuracies, but also qualitatively different dynamical behaviors on long length and time scales.

2.3. Defects in pattern-forming systems. Pattern formation in nonequilibrium systems is commonplace, and considerable effort has been devoted to characterizing patterns, selection mechanisms, and instabilities in such systems. [1] More recently, much work has focused on the formation and evolution of localized defects in regular patterns. A prototypical pattern-forming system, such as Rayleigh-Bénard convection of fluids, is seen to enter into an exotic state of *spiral defect chaos* as it is driven sufficiently hard by an external temperature gradient. [2] A snapshot of spiral defect chaos in a Rayleigh-Bénard experiment by Morris, Bodenschatz, Cannell and Ahlers, captured using shadowgraph techniques, is shown in figure 3, and various movies can be found online. [13] The dynamics of this system are driven by these localized spiral features, although an understanding of the details of those dynamics is yet to be achieved.

Simulations of the three-dimensional Navier-Stokes equation can be carried out to probe the dynamics of spiral defect chaos, but often simpler model systems are investigated to enable more thorough investigation of defect-mediated dynamics. A prototypic system for the study of defects in pattern-forming systems is the Complex Ginzburg-Landau (CGL) equation. This model describes the time-evolution of a complex order parameter field $\psi(\vec{r}, t)$:

$$\partial_t \psi = \epsilon\psi + (1 + ic_1)\nabla^2\psi - (1 - ic_3)|\psi|^2\psi \tag{1}$$

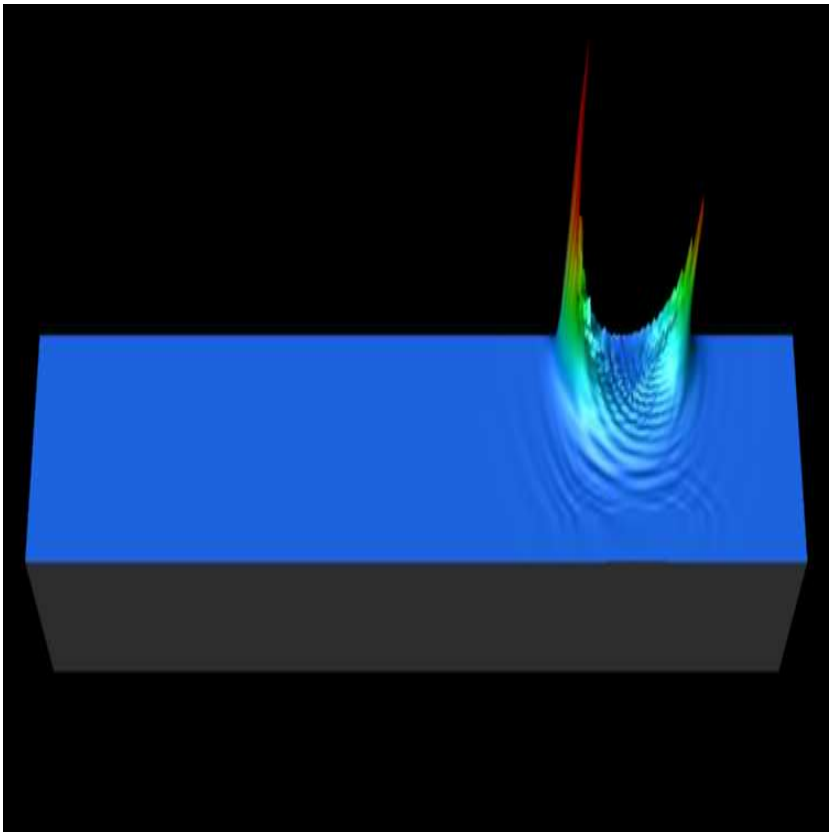

FIG. 2. *Snapshot of propagating slip pulses in a model of an earthquake fault.*

In certain parameter regimes, vortex line defects spontaneously form, migrate and entangle, driving a defect turbulent state. Furthermore, dynamical transitions between qualitatively different states occur as a function of system parameters. Simulations of a three-dimensional CGL equation by David Egolf[14] demonstrate the complexity of the vortical defects. Figure 4 illustrates isosurfaces of the amplitude of the complex order parameter field, encompassing lines of phase defects. These phase defects exist only at those points in space where the amplitude of the field is zero; the formation of the defects is driven by strong deformations (gradients) in the phase field.

2.4. Dislocation dynamics and plastic flow in solids and driven periodic media. A specialized instance of dislocation dynamics in pattern forming systems involves the dynamics of plastic flow. While dislocation dynamics have long been investigated by engineers studying crystalline solids, there is a recent surge in interest in understanding the fundamentals

FIG. 3. *Spiral defect turbulence in Rayleigh-Bénard convection (from ref. [13]).*

of plastic flow through the investigation of other sorts of periodic media, often because signatures of plastic flow are more experimentally accessible, or because external parameters can be conveniently tuned to probe the system. These include vortex lattices in Type II superconductors [15] and sliding charge density wave (CDW) conductors [16][17]. Of particular interest are: (1) the relationship between the detailed character of dislocation motion and the macroscopic signatures of such motion, and (2) the nature of dynamical phase transitions between qualitatively different states as system parameters are varied.

Earlier models of CDW conduction treated the CDW as a purely elastic medium, not capable of tearing or otherwise deforming plastically. [18] Within these models, the time-averaged velocity of the CDW is spatially uniform, with no portions of the CDW moving more rapidly or more slowly than others. It has been recognized, however, that such models are both ill-defined in the limit of infinite system size and incapable of describing

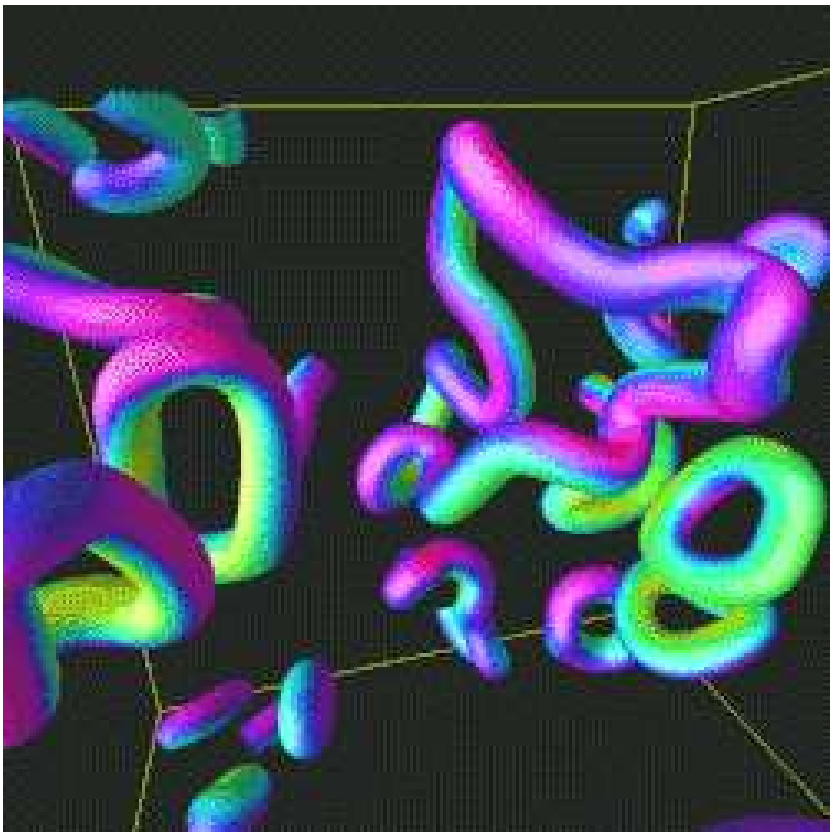

FIG. 4. *Vortex defects in the 3D Complex Ginzburg-Landau equation (from ref. [14]).*

$1/f$-like broad band noise (BBN) current spectra in sliding CDWs. In analogy with the defect turbulence described above in the context of pattern-forming systems, it is plausible that a similar defect-mediated spatiotemporal chaos associated with plastic deformation of the sliding CDW could give rise to BBN in a suitable model of such a system.

The model of Balents and Fisher provides a reasonable starting point for such an investigation. [16] This model, derived largely on grounds of order-parameter symmetry (and hence quite similar to the CGL equation described in the previous section), describes the evolution of the complex CDW order parameter ψ in the presence of random, quenched disorder.

$$\begin{aligned}\partial_t \psi = [D\nabla^2 + v\partial_x + M + r(\mathbf{x}) + i\omega_0 + iF(\mathbf{x})]\psi \\ -u\psi|\psi|^2 + \xi(\mathbf{x},t)\end{aligned}$$

In this model, $r(\mathbf{x})$ and $F(\mathbf{x})$ are quenched, uncorrelated random fields

and $\xi(\mathbf{x}, t)$ is a complex stochastic noise term, as is typically present in Langevin models.

I have carried out some preliminary investigations of this model, primarily in two dimensions. Upon integration of the Balents-Fisher equation of motion, I have found that, in certain parameter regimes, CDW defects are prevalent, and associated with aperiodic evolution of the CDW current. The defect structures in the sliding CDW tend to be more extended than in the CGL equation without disorder. In two dimensions, CGL defects are point-like, whereas CDW defects are more line-like; while in three dimensions, the CGL gives rise to line-like vortex tubes such as those shown in figure 4, whereas it is expected that the CDW would exhibit plane-like sheets of defects. This appears to be because a characteristic length scale of the effective disorder (ξ_d) is set by the combination of the intrinsic pinning strength and the external driving field. Regions of size ξ_d tend to move at different time-averaged velocities, producing large phase strains along the boundaries of those regions. This reduces the CDW amplitude along those boundaries, producing extended defect structures not unlike grain boundaries in crystalline solids.

A snapshot of the CDW phase $\phi(\vec{r})$ and amplitude $A(\vec{r})$ is shown in figure 5. The features in the plot of the CDW amplitude $A(\vec{r})$ reflect the regions of diminished amplitude; these regions tend to demarcate different velocity-coherent patches of the CDW. The demarcations are not static, however, but migrate and meander over time.

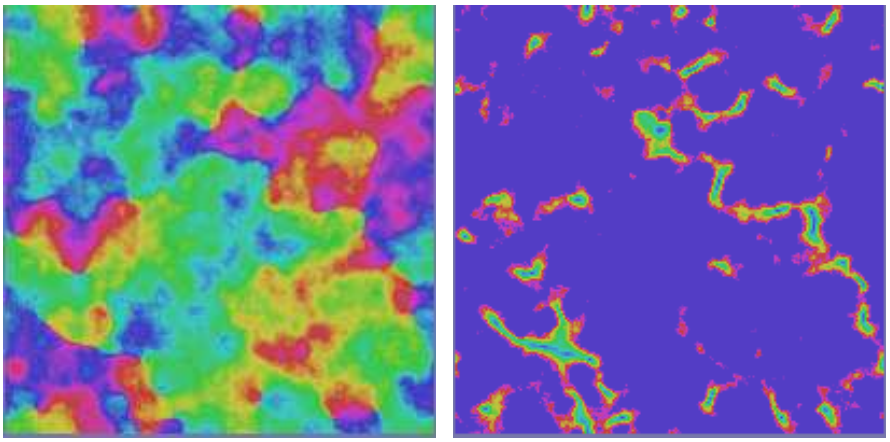

FIG. 5. *Snapshot of the phase field $\phi(\vec{r})$ (left) and the amplitude field $A(\vec{r})$ (right) for a plastically flowing two-dimensional CDW.*

The reduction of plasticity at higher driving fields is due to the relative weakening of the quenched disorder field, as compared to the external drive. It is expected that some sort of dynamical phase transition to a more ordered sliding state may occur at sufficiently large drives as the dis-

order becomes less relevant, but there is currently a debate as to whether that high-velocity phase may be a "moving solid", "moving Bragg glass", or "moving smectic". Nothing from the preliminary studies that I have carried out on this system will resolve that debate. From a computational point of view, however, especially regarding the utility of adaptive mesh refinement methods, it should be recognized that such a debate places perhaps the most demanding requests on a simulation as can be imagined; one is asked to resolve between different scenarios involving the growth and divergence of a dynamical correlation length which is roughly set by the spacing between localized coherent structures (dislocations), which themselves must be resolved faithfully in a simulation, and which are migrating chaotically in time.

3. Problem-solving environments for coherent structures. Understanding the complex spatiotemporal dynamics of coherent structures in driven, nonlinear systems is a nontrivial task, both theoretically and computationally. In developing software environments to facilitate such understanding, one must effectively integrate numerical methods, complex data structures, visualization environments, data and metadata management packages, symbolic mathematics, image processing, etc. Typical computing paradigms which emphasize batch processing of codes containing "numerical kernels" as separate from (and typically more important than) "postprocessing" and visualization tend to inhibit advances in problems that require interactive and visual exploration of dynamical processes such as is the case with coherent structures in nonlinear systems. The IMA Workshop contained several talks which demonstrated, either explicitly or implicitly, the value of integrating numerical "processing" and visual "postprocessing" in a single environment. James Quirk's talk on the AMRITA system described one approach to such an environment, and Matt Choptuik's talk on SAMR for numerical relativity clearly demonstrated the essential value of interactive problem solving environments to support the investigation of the dynamics of localized structures.

Furthermore, software design for complex problem domains must balance the need for flexible and extensible control while shielding the programmer and/or user from inner details. Developing a completely insular "black box" for SAMR in complex dynamical systems is a dubious goal. An important lesson evident at the IMA Workshop is that support for SAMR is very hard to generalize across problem domains, and needs to provide support for the researcher to apply heuristics or very specialized numerical methods. At the same time, however, the underlying algorithms and data structures for SAMR are sufficiently complex that there needs to be substantially better abstraction and encapsulation of various elements of SAMR methods. The growing use of object-oriented programming methods to address the challenges of SAMR methods reflects the recognition that control must be balanced with encapsulation. In addition, object-

oriented methods are extremely useful for encapsulating low-level details arising from the implementation of adaptive mesh methods in parallel architectures.

3.1. Multiscale modeling. The increasing power of supercomputers and a growing interest in multidisciplinary collaborations has led many groups to undertake multiscale materials modeling, to incorporate more accurate small-scale physics into large-scale materials computations. In many cases, simulations of phenomena at one scale suggest the need for feature extraction and abstraction at a larger scale. Understanding the collective dynamics of interacting localized defects is encumbered by the need to simulate large portions of the system that exhibit rather simple structure or dynamics. The ability to represent only the defects themselves and their interactions with each other may enable one to apply techniques from statistical mechanics to understand better the collective response of the system.

Efforts are underway to develop both a better qualitative understanding of the role of defects and other coherent structures in controlling the dynamics of nonequilibrium systems, as well as a better quantitative understanding of the interactions between coherent structures, for use in reduced order models. For example, detailed comparisons between large aspect ratio convection experiments and large-scale, parallelized Navier-Stokes simulations are providing quantitative information about the dynamics of spiral defects and other structures in Rayleigh-Bénard convection. [13] (Even so, advances need to be made to better integrate image processing of experimental data into the broader simulation and data analysis framework.) Exciting developments in the simulation of plasticity in crystalline systems are unfolding from the development of simulation models which treat only the dislocations themselves (as line-like objects) and not the crystalline background from which them emanate. [19] Additionally, the application of various mathematical methods for the extraction of coherent structures from time-evolving flows is becoming more widespread. [20]

In order to extract coherent structures for the development of reduced order models, or to explicitly couple different models at different length scales, one needs a software environment that can adapt the representation and implementation of coherent structures to various contexts. In coupling atomistic simulations of microscopic phenomena with continuum models of macroscopic materials, for instance, one may need to represent somehow the defects that arise naturally in an atomistic simulation (dislocations, voids, etc.) as they migrate into a region of the material treated by a continuum model, or otherwise treat such atomic-scale structure faithfully. [21] Adaptive mesh refinement strategies can play an important role both in terms of providing accurate, highly-resolved calculations of the structure and dynamics of coherent deformations, and in helping to manage the internal details of transforming representations between different contexts.

3.2. Interactive simulation, prototyping and analysis. Advances in new algorithmic and application areas, such as those involving the use of SAMR methods to study coherent structures in nonlinear systems, require an environment where researchers can conveniently explore and prototype various algorithms, strategies, refinement criteria, etc. The success of Matlab, for example, as an interactive problem-solving environment for linear algebra is undisputed; that success arises largely from the fact that Matlab allows users to create and manipulate matrices at a high level of abstraction, without worrying about low-level implementation details. Unfortunately, Matlab does not conveniently support richer data structures such as those needed to describe adaptive mesh hierarchies. But just as fortunately, novel software engineering tools are becoming available and widely used to enable the development of more appropriate problem-solving environments for complex methods such as SAMR.

A promising approach for the construction of flexible, interactive, integrated problem-solving environments involves the use of extensible scripting languages augmented by compiled extension modules. In particular, object-oriented scripting languages – such as Python[22] – can allow one to create interactive, interpreted interfaces to compiled object-oriented codes (such as C++ libraries used to implement numerical methods for PDEs). This approach, using scripting languages to provide more convenient runtime access to compiled objects, is beginning to receiving considerable attention within the scientific computing community. [23]

I will illustrate this approach using pieces of the PDESolve library from Beam Technologies, Inc. [24], although the approach itself is more broadly applicable. PDESolve is a C++ class library which provides a high-level syntactical interface to partial differential equations (PDEs), allowing users to manipulate differential operators, scalar and tensor fields, solvers, etc. (PDESolve does not directly support SAMR methods at this time, although such methods could be built out of the pieces provided by the library.) A similar project could endeavor to develop an interpreted interface to some of the C++ libraries pertinent to SAMR methods, such as DAGH[25], KeLP[26], AMR++[27], etc.

Developing an interpreted interface to a compiled library such as PDESolve is greatly facilitated by SWIG, an automated wrapper-generation tool written by Dave Beazley [28]. SWIG removes most of the tedium typically associated with writing interface wrapper code for compiled libraries, and is capable of outputting scripting language interfaces for a number of languages besides Python (e.g., Tcl, Perl, Guile). SWIG also can generate "shadow classes" for scripting languages such as Python that support object-oriented programming; as a result, one can manipulate classes within the Python interpreter that mimic the underlying C++ classes that are carrying out the bulk of the numerical computation.

A fragment of PDESolve code, written in C++, might look like this:

```
#include ``PDESolve.h"
int main(int argc, char **argv)
{
  SpatialDomain domain =
       SpatialDomain(0., 1.) * SpatialDomain(0., 1.);
  FDMesh grid(domain, FDMeshSpec(32) * FDMeshSpec(32));

  DiffOp dxx(2,0,6);
  DiffOp dyy(2,1,6);

  Function u(2, Scalar);

  Expr model = dxx*u + dyy*u;
```

Objects representing spatial domains, finite-difference meshes, differential operators, unknown functions, etc., are constructed and ultimately assembled to solve a specified PDE. A Python interface to such a library, however, allows one to manipulate these objects at run-time within the Python interpreter. The equivalent fragment of Python code appears as follows:

```
from PDESolve import *

domain = SpatialDomain(0., 1.) * SpatialDomain(0., 1.)
grid = FDMesh(domain, FDMeshSpec(32) * FDMeshSpec(32))

dxx = DiffOp(2,0,6)
dyy = DiffOp(2,1,6)
u = Function(2, Scalar)

model = dxx*u + dyy*u
```

I hope that the utility of such an approach is obvious. Once interpreted interfaces to complex objects such as adaptively refined grid hierarchies, error estimators, and time-stepping algorithms are developed, one can experiment with different SAMR strategies within the confines of the interpreted Python environment, bringing in support (in the form of dynamically loaded Python modules) for visualization, database interfaces, internet connectivity, etc., as needed.

In addition, since Python itself is a powerful object-oriented language, one can in principle relegate a good deal of high-level abstraction to the Python overlayer rather than embedding it in the C/C++ underlayer. This may be especially convenient for SAMR, since generalizations across prob-

lem domains appear to be particularly problematic. If sufficiently generic low-level abstractions are provided, then the rapid prototyping capabilities of a language like Python could enable the development of application-specific class hierarchies without requiring those specializations to be included in the underlying library.

4. Summary. Structured adaptive mesh refinement is a powerful technique that has the potential to enable breakthroughs in a number of complex problems in science and engineering where the dynamics of localized coherent structures dominates the response of a system. The dynamics of such systems will provide an important testing ground for broadly useful software for SAMR. But such systems also stress the need for adaptive software along a number of fronts, not just in the numerical solution of PDEs. Adaptive software components for feature extraction, image processing, multiscale modeling, rapid prototyping and interactive steering all need to be integrated with SAMR numerical kernels in order to produce truly useful problem-solving environments for understanding the dynamics of localized coherent structures in nonlinear dynamical systems.

5. Acknowledgements. I would like to thank the organizers of the IMA Workshop on Structured Adaptive Mesh Refinement Grid Methods for putting together a very enjoyable and productive workshop, and for inviting me to present some of my work there. I would like to thank Farid Abraham, Eberhard Bodenschatz, and David Egolf for allowing me to incorporate some of their work in my own discussions of coherent structures. And finally, I would like to thank the Cornell Theory Center for enabling and encouraging me to work across a number of disciplinary boundaries in science and computing, many of which are represented here.

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