Joan Adler - Research Statement - 2017 updates are bulleted.

I have five primary foci in a research program based on development and application of numerical algorithms, with a substantial vizualization component, to model physical phenomena.

1. Critical phenomena

One of the best approaches to understand critical phenomena at a phase transition (PT) is the method of exact series expansions. A convergent series expansion of the exact solution of a model, such as an Ising or percolation model, can be extrapolated into its critical region to deduce critical exponents and temperatures. Popular methods to do this include a group of transformations known as AMP (Adler/Moshe/Privman) which are variations of Padé approximants, that take into account corrections to scaling. They are generally deployed with 3D graphs of approximant surfaces, see Fig. 1. The AMP method was developed at the Technion, while I was a Lady Davis postdoctoral fellow and applied further during my time at Tel Aviv University and then in three successive GIF collaborations with groups in Germany on my return to the Technion in 1990. Some 48 papers, including invited reviews [R-1,2,5,7] (numbers in brackets refer to papers in my CV, R indicates a review and C a conference paper) and two Technion graduate student theses have resulted from these studies. My results are quoted extensively in monographs, textbooks and several summary tables in Wikipedia.

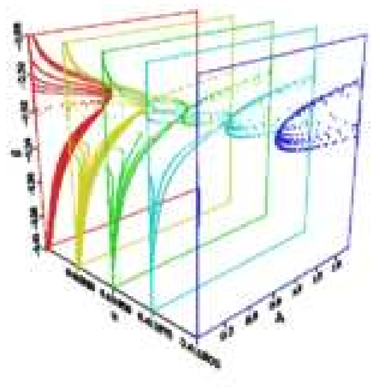

Fig. 1 AMP visualization for 3D Ising model from [87].

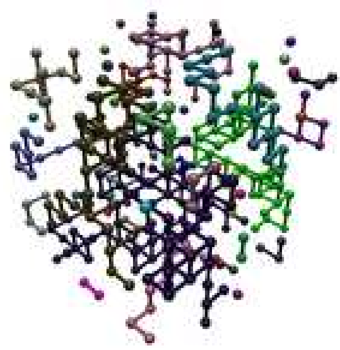

Fig. 2 3D Percolation clusters.

2. Percolation

Percolation is a model of a system where sites (or bonds of a lattice) are randomly occupied, with probability p. When p reaches a critical value, p_c, a connected cluster of occupied sites (bonds) occurs and the system undergoes a PT. I have applied series expansions and renormalization group methods as well as large scale Monte-Carlo simulations to percolation, and co-edited a book "Percolation Structures and Processes" that although currently out of print is under consideration by two different publishers for a new version with an updated introduction. Recent activity in my group has centered on 3D percolation with several undergraduate projects, one with a WebGL virtual reality site (Liran Sharir, Fig. 2 on the previous page) and one with a Hebrew educational website and analog demonstrations. I have worked on percolation continuously since my undergraduate project in 1974, until the present day.

PERCOLATION VARIANTS: Two features that distinguish percolation models are symmetry (isotropic or directional) and correlations in the randomness. Directed percolation, where connection is possible only in one direction is in the same universality class as Reggeon field theory, which led us to the AMP methods, mentioned above. Bootstrap percolation (BP), is a correlated percolation model where sites that do not have enough neighbours (at least m neighbours are needed) are removed. The culling process is a random cellular automaton. There are interesting critical phenomena and finite size effects, in these models, much studied in the mathematical community. My review [R-3], on BP is widely cited, especially in the last 5 years. I also proposed and developed analytic results for a model I called diffusion percolation which is a BP inverse. The original article [32] is again much cited recently and is currently being used to model growth in colloid mixtures in materials science.

FUTURE PLANS: Isotropic percolation - in the percolation heydays in the 80s and 90s, much attention was focused on cluster structure in two dimensions and the nature of the connectivity (blobs, links, etc). Less attention was paid to three dimensions, because it was hard to model cluster structure in large enough 3D systems, and very hard to visualize this. Questions concerning the nature of the connectivity, such as are there multiply connected sites, or are parts of the cluster connected by a simple backbone, have arisen in biophysical applications to tissue breakdown and decay. Hence my recent activity in the virtual reality sphere, and I am about to start a new project to collect and analyze data on the nature of 3D clusters, at and above the phase transition.

FUTURE PLANS: Correlated percolation - I have proposed several condensed matter applications of BP to such diverse systems as orientational order in solid molecular hydrogen [32,C-13] and preparation of smooth diamond surfaces for quantum computers [130]. The former may exhibit a quadrupolar glass phase and I plan to return to this system in the near future now that computational advances enable study of larger systems.

• Percolation updates will be described in the Computational Physics Education section below.

3. Atomistic simulation and vizualization

In the early 90's I re-evaluated my research program and moved intentionally towards interaction with condensed matter laboratory experiments. Armed intially with the computational techniques of simulated annealing from statistical physics and molecular dynamics and later adding density functional theory (DFT) combined with constant interactive visualization, I began a program of modelling a wide range of systems, generally with one or more graduate students and an experimental partner. Several semiconductors [13,55,67,69,71], ceramics [102-3], diamond [48,86,89,91-2,96-7,99,101,111-2,119,122,124-5,127,130,139], metals [100,107,109,110,120-1,133] and more recently nanotube systems [128-9,131-2,134-6] were selected. These have been central to my research in the last 20 years, and led to some 20 graduate student theses. I developed a custom-designed 3D visualization code AViz for these projects. I have recently collaborated in the design of an interopability framework called SimPhoNy, which is an EU NMP FP7 project concerning multiscale phenomena in nano and micro systems, together with my former graduate student Adham Hashibon of Freiburg.

• The SimPhoNy project has been successfully concluded, with multiple publications. A new Horizon2020 project, known as ENITMO, (ENgaging the material industry in the use of Tools for multiscale MOdelling) with some of the same participants, and including Simon Brandon of Chemical Engineering, Technion is now in advanced planning stages.


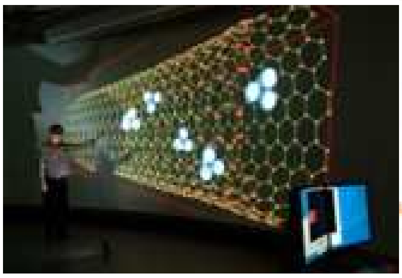
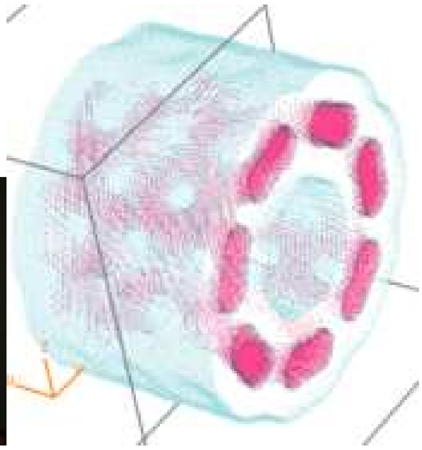

Fig. 3 Vanadium melt [109]. **Fig. 4** CH_4 flow [128]. **Fig. 5** Electronic density [138].

HIGHLIGHTS: Selecting these is difficult. One series of studies with E. Polturak, has covered melting phenomena in metals, An example from a study of vanadium where we demonstrated pre-melting surface phenomena is shown in Fig. 3. The many diamond projects have covered the first explicit observation of the formation of the split interstitial defect, modelling the growth of graphitic planes in damaged diamond (hence disturbing its insulating properties), effects of the heat spikes in diamond, formation of amorphous structures, conditions for growth of nanodiamond and recently formation of nitrogen-vacancy centers. Direct comparison between simulated phonon spectra and Raman spectra enabled identification of point defects in diamond. The diamond projects branched into modeling of flow in nanotubes, and collaborations with Juelich; Fig. 4 shows a stereo version of AViz and movies of this appear in the PRACE publicity videos. The nanotube modeling was extended to study the electronic density of the nanotubes, calculated with DFT [138], and visualized with an off-label AViz dot approach, see Fig. 5.

• Progress here has included electronic visualization of nanotubes with attached objects, and a manuscript is in preparation.

FUTURE PLANS: All these studies have possibilities of continuation, with demand from old and new experimental partners both local and overseas exceeding any realistic expectations of being met. My inclination is towards further effort in the direction of interopability of the simulation codes and the visualization of the results, and a project concerning electronic density visualization of some carbon molecular systems that are not nanotubes. My immediate goal is to complete my 3/4 written book on "Visualization for materials science", commissioned by Taylor and Francis two years ago.

4. Computational physics education

I have developed an approach to teaching algorithms and application of computational physics via guided examples, with a heavy visualization component. I have given invited talks, colloquia and many conference presentations on this approach, especially presenting the final class projects where I often help students model a topic from their own research or a topic in undergraduate education that they can explain with animations. Conference proceeding papers [C-13,17,20-8] describe my approach and some of the student projects. Of special importance are the stereo animations of H atomic wave functions [C-24,26], already in use in undergraduate physics classes at Technion and overseas.

FUTURE PLANS: Due to rapid developments in computer hardware and software this educational material has to be frequently updated. Last year I added a DFT component to my course material and I am in the process of adding an introductory module on GPU use, part of which has just been submitted for publication, following a well received talk at CCP2016.

• The GPU manuscript has appeared, and now one on simulation of liquid crystals and colloids is submitted from CCP2017 in Paris.

• Three recent educational achievements are:

i An analog model for percolation, to be installed in the department and used for visiting children. (Fig 6.)

ii An invited Master Class on Computational Physics Education at HSE in Moscow. (Fig 7).

iii Material for High School lectures for an introduction to percolation with the "Percolation Bingo " game, given in December at the LIGHT Spikes/FIRST meeting in Lod and ready for more extensive distribution.



Fig. 6 Percolation display. **Fig. 7** LSE class **Fig. 8** Nanotube + ring.

5. Application of statistical physics algorithms outside condensed matter, especially to optical systems

There is a deep analogy between the roughening transition in crystal growth [74,83, 85,C-28] and the phasing of a multimirror telescope. In fact, they have similar Hamiltonians. I found that expertise from simulated annealing of crystal systems into their groundstates enabled me to achieve rapid phasing of adaptive optics systems. Papers [49-50] describe several projects of this type for both telescopes and microscopes. The most recent of these [137] was a parallel study by myself and student Irina Paykin who built models and student Lee Yaacobi and Dr Erez Ribak who applied our algorithms to a laboratory system.

FUTURE PLANS: The above models were developed on an ad hoc basis. I plan to set up a framework that will enable this phasing to be carried out for various models from a single adaptable code that will include a completely new vizualization module.