Second Annual Progress Report

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Part A - Research Results

A.1 Scientific Highlights

These are presented by task, though some could be put under more than one task and others do not fit perfectly. (The coodinator apologises that this section overruns the allowed space of 2 pages: he did not have time to condense the ample contributions and put them in a uniform style. The relative space taken by each task should not be taken as an indication of its significance.) Throughout the report, "DB" stands for "discrete breather".

T1 Breather existence Explicit estimates for continuation of DB came out in print this year [K], as well as a variational proof for the existence of hard DBs in FPU lattices and models with acoustic phonons in any dimension [AKK]. Existence proof of hard DBs in FPU lattices constructed by a reduction to centre manifold came out [J] and is being extended to more general situations (G.James), and applied to existence of breathers in diatomic chains with arbitrary mass ratio (G James & P Noble). Evidence for existence of DB in realistic models for hydrocarbons was found numerically [KA01]. An algebraic method has been proposed to construct analytically DBs in 1D chains [Ts] and numerical methods are being investigated for finding DB in 1D nearest neighbour chains as homoclinic orbits of a 2nd order recurrence relation on a loop space (Bergamin, Kadelburg & MacKay). Existence of solitary waves in some 2D lattices was proved [FrM1], as well as atomic-scale localization of high-energy solitary waves on lattices [FrM2]. Existence of DBs has been shown numerically in dipole-dipole chains with long-range interactions and curvature, and their linear stability and new properties have been investigated [ACMG, ACG, CGMM]. Existence of DB in spin lattices has been proved in [ZFF] and reviewed in [FZ]. Exact quasiperiodic breathers have been studied in dissipative (Josephson junction) systems with external DC bias [FMFSU]. Existence of quasiperiodic breathers in systems having integrals of motion independent of the Hamiltonian was proved [BV]. A thorough study was made of spatial decay properties of breathers in lattices with no linear dispersion [DEFT].

T2 Breather Quantisation and T3 Coupled quantum rotors or spins The analysis of the dynamic structure function $S(\mathbf{Q}, \omega)$ measured with single crystal of 4-methylpyridine in terms of the extended sine-Gordon theory is in progress in Thiais. A theory of quantum discrete breathers has been proposed, which in particular discusses the interpretation of Fillaux and Carlile's experiments on 4-methyl pyridine and proposes a tentative alternative [M2]. The angular probability densities for the methyl deuterated lithium acetate dihydrate have been measured with the single crystal neutron diffraction techniques. A new dynamical model is proposed to account for the interplay of methyl dynamics and crystal structure, with special attention focussed on the deuterium induced phase transition [NCF]. A theoretical study of energy and momentum tunneling in a system of two coupled quantum rotors has been completed. This is both an abstract model for rotational degrees of freedom in molecules and a paradigmatic model for quantum rotobreathers in extended systems [DF]. Exact energy levels for a finite no of quanta (up to 5 or 6), and a finite number of sites (up to 13), for QDNLS, QAL, QSalerno, have been calculated (Eilbeck, Salerno & Scott).

T4 Breather mobility An abstract framework for understanding the occurence and motion of approximate travelling discrete breathers in Hamiltonian chains of oscillators has been developed. The concept of Peierls-Nabarro barrier for DB is made clear in this framework [MS02]. Work is also continuing on generic non-persistence of exact travelling DB (Rothos & MacKay). Analytical conditions for breather mobility between two sites were determined in [AKMT01] and called Targeted Energy Transfer (TET): the DB oscillates periodically between the two sites. Using the analytical conditions, TET was detected and tested numerically in some complex models [KAT]. The existence and properties of static and moving breathers have been studied in a DNA model with nearest-neighbour interaction, due to the stacking of the base pairs, and long–range interaction, due to the dipole moment of the bond within each base pair [CAGR]. Work on travelling DB in cuprate layers as a possible mechanism for HiTc has continued (Eilbeck & Russell). In the related area of nonlinear waves, a study of hyperelliptic ζ-function solutions in the integrable massive Thirring model, a field theory model, has been completed [EEH]. A number of advances have been made in understanding how generalized Weierstrass Elliptic functions of higher genera can be used to solve nonlinear wave equations [AEE]. Normal form techniques have been used to obtain the nonlinear Schrödinger equation as a modulation equation for moving quasiperiodic breathers in FPU–type systems [BCP]. DB mobility has been investigated in curved chains [RSIT, TIS]. They introduced a modified Fermi-Pasta-Ulam model and demonstrated that DBs change their mobility properties while in curved parts of a polymeric chain. The basic result is that in the regime where breathers are mobile in the rectilinear chain, DBs remain intact in curved, semicircular segments of the polymer while propagating freely with different velocities. Their motion is governed locally by mechanical conservation of energy. These results were extended in curved polymer chains with first and second neighbour interactions as well as with local on-site potentials. Their models, that are the simplest minimal models for biomolecules, demonstrate that breathers are very robust and survive even dramatic geometric shape changes.

T5 Phonon-breather interactions and self-localisation Standing phonons have been constructed in Klein Gordon chains as multibreathers and numerically analyzed [MJKA02]. It was shown that any small nonlinearity is sufficient to make the standing wave unstable which might be strong or weak for some incommensurate standing waves [MJKA]. The thermalization of the system following the instability has also been analysed and involves sometimes transient DBs [JMAK]. The origin of puzzling solutions called Phantom DBs found only in relatively small finite systems has been elucidated [MJAK02]. We have also investigated the energy relaxation process produced by thermal baths at zero temperature acting on the boundary atoms of chains of classical anharmonic oscillators [PLL]. We discuss the mechanism yielding such solutions and also explain why it is crucially depends on the boundary conditions. Relaxation phenomenon in the 2D FPU emphasizes the role of the threshold for the creation of breathers. Moreover, the decrease of the mobility of breathers slows down the relaxation. The role of breather creation in a phenomenological model dedicated to the study of polymers ageing properties has been studied. Consequences for the so-called alpha and beta relaxations characteristics of real polymers are investigated. A shell model of turbulence involving creation, interaction and decay of breathers was studied. Analogies and differences between breathers and vortices in fluids are discussed, and their consequences on the non gaussian fluctuations of the probability density functions are discussed. Localisation of energy in the $N-H$ stretch of crystalline acetanilide has been observed [EHS]. A role of self-trapped states in conformational instability of biopolymers has been investigated and a new mechanism for polymer folding has been proposed [MGCK]. We have studied analytically the behavior of the largest Lyapunov exponent for a one-dimensional chain of coupled nonlinear oscillators, by combining the transfer integral method and a Riemannian geometry approach. We characterize it as a dynamical indicator of a phase transition [BD] We have studied an analytically tractable model with long-range interactions for which an out-of-equilibrium very long-lived coherent structure spontaneously appears. The emergence of the structure is explained using the associated hydrodynamical equations, whereas we get an explanation of the very long time stability of the bicluster: this out-of-equilibrium state corresponds to a statistical equilibrium of an effective mean-field dynamics [BBDR].

T6 Randomness and nonlinearity 1) Spatial randomness: The interplay between nonlinearity and randomness in 2-dimensional systems was studied in [CAPR]. Properties of non-

linear impurity modes and their stability have been studied in the generalized Schrödinger equation [SKBRC]. Conditions for breathers travelling over an a impurity have been found [CPAR-II].
2)Temporal randomness: The survival of breather mobility across bending points in polymers when temperature is considered is observed in [RSIT, IST, TIS]. The thermalization of standing phonons leading to transient DB is studied in [JMAK]. Work is still in progress on nonlinear conductivity of CDW materials by thermal nucleation of pairs of discommensurations (Baesens, MacKay, Floria & Sancho).
3)Application to DNA: Mobility of polarobreathers is observed to survived to weak diagonal and structural off-diagonal disorder in a 3D DNA-model.

T7 Slow Relaxation After the first success in using time–dependent perturbation theory for deducing the existence of different phases in the energy release process produced by thermal baths at the boundaries [PLL], further progress has been achieved for the 2D case, where the additional effect of the existence of an energy threshold for breather activation has been identified and described [PLLa].

T8 Polarons Existence of multihump solitary waves has been shown in the Davydov model [OMKGC]. A model 1-D system which describes two quasi-particles interacting with a nonlinear lattice has been studied. The quasi-particles are treated quantum mechanically, whereas the lattice is treated classically. For a range of model parameters, they find pairing between the two quasi-particles. The dynamical stability of such pairs show a range of interesting regimes, with possible applications to models of HTSC [CEMR]. We studied the semiclassical Holstein model with a hard nonlinear on-site potential in one, two and three dimensions. Using stationary solutions, we obtained the ground-state phase diagram as a function of the parameter characterizing the nonlinearity as well as the electron-phonon coupling. The dramatic reduction of the polaron effective mass is the most characteristic effect of the lattice nonlinearity. We studied the many quanta problem of an intra-molecular vibrational excitation that interacts with optical phonons. In the adiabatic limit we calculate numerically the ground state energy and the corresponding wave functions for N vibrational quanta. In the one-dimensional case we find strong red-shifts in the overtone spectra and an increasing spatial localization as the number of quanta increases. Through model parameter fitting we achieve very good quantitative agreement with experimental Resonant Raman scattering measurements in the quasi-one-dimensional charge transfer solid $PtCl$. Accurate analytical expressions for the red-shifts are obtained through the anticontinuous limit of the many-quanta energies. Charge transport mediated by polarons has been investigated for in variant of the Holstein model, taking in account the helicity and the disorder.

T9 Josephson arrays Interaction of discrete breathers with linear cavity modes of Josephson junction ladders have been studied theoretically in detail by Dresden group [MFFZP]. These interactions have been experimentally observed in Erlangen, as resonant step in the I-V characteristic of Josephson junctions ladders [SBU]. Incommensurate resonant breather states in Josephson junction ladders have been also observed in experiment and theoretical studied [FMFSU]. A detailed theoretical study of the existence, stability and resonance behavior of breather-like states in small Josephson system (3-junction cell) has been done by Dresden group [BFF], [FFB]. Such cell of Josephson junctions has been prepared and is currently under investigations by Erlangen group. In recent experiments the predicted resonant states in the cell have been observed. Effects of the ac drive on the fluxon motion have been studied [SZ].

T10 Friction and nonlinear conductivity Topological defects and dislocations in strongly anisotropic crystals are shown to propagate freely with stationary profile and velocity [SKCZ]. We addressed the problem of heat conduction in 1-D nonlinear chains; we showed that, acting on the parameter which controls the strength of the on site potential inside a segment of the chain, we induce a transition from conducting to insulating behavior in the whole system. Quite remarkably, the same transition can be observed by increasing the temperatures of the thermal baths at both ends of the chain by the same amount. The control of heat conduction by nonlinearity opens the possibility to propose new devices such as a thermal rectifier [TPC].

T11 Proton transfer 1 - Hydrated Protein: A model of two-dimensional water is studied in order to analyze recent dielectric measurements on protein hydration water. The frustration introduced by the coupling of the water molecules to the protein surface prevents a true crystallization and induces a glass transition. The results suggest that two-dimensional water, which can be probed by dielectric measurements, could be an interesting system to study the glassy behavior of water [P, P1, CP]. New dielectric measurements with hydrated powders are underway.

2 - Proton Transfer in KHCO3 and Benzoic Acid: New evidence for proton transfer along hydrogen bonds were analysed in Thiais and a purely quantum mechanical mechanism has been proposed to account for the proton transfer rate at any temperature [FLR]. We have obtained new evidence for localized modes in the KHCO3 crystal [IKKSYBF].

3 - Breathers or Proton Hopping in L-Alanine: New infrared observations of the NH3 torsional mode at 490 cm-1 demonstrate the existence of a splitting below 220K, a strongly temperature dependent intensity and the presence of an overtone at 950 cm-1. These unusual properties are well taken into account within the theory of vibrational polaron [BVSBE], but could also result from some structural instability. No phase transition could be deduced from our precise birefringence study (in agreement with previous crystal structures at RT and 20K), but a strong depolarization of the transmitted light occurs, indicating a subtle symmetry breaking [BVSBE]. A new Raman scattering investigation confirms a singularity of many external modes and of the NH3 torsion at 220K. The interplay of the librons at 40 and 48 cm-1 is also confirmed, and assigned to the strengthening of the H-bonds on cooling which induces an alteration of the eigenvector for these modes. A random proton exchange on the ammonium group could explain the instability at 220K [VYBS]. High resolution X-ray diffraction is now planned at the ESRF.

4 - Low Frequency Dynamics of N-MethylAcetamide: Following our investigation of the crystallographic structure by neutron diffraction [EBall], quasi-elastic neutron scattering study of NMA and deuterated isotopomers shows a dynamical rotational disorder around the C-C axis. Activation energies for the random hopping of methyl protons are significantly different for each methyl group (50 mev and 86 meV) showing that the reorientations of the methyl are highly dependent on the local arrangement [RBB]. Inelastic neutron scattering studies at low energy are now underway.

T13 DNA and Proteins Progress in the statistical mechanics of DNA melting included (i) the systematic study of static correlations and scaling, and (ii) understanding the role of soliton-like excitations in the more general category of one-dimensional thermodynamic instabilities [DTP]. In addition, we have performed preliminary molecular dynamics simulations of the critical dynamics of DNA melting and melting transition of DNA has been studied by a simple mechanical model which includes the double helix geometry [BLP]. The role of DNA curvature and rigidity on the existence,stability and mobility of breathers have been investigated [AK02b, ACMG, ACG, RSIT, TIS, IST, CAGR] and static and moving breathers in curved alpha-helix proteins have been studied. A model for the diffusion of RNA polymerase along DNA has been proposed [BPPS]. Studies on proteins have been devoted to various aspects of electron transfer through nonlinear effects and polarons. A model of ultrafast electron transfer between a dimer of bacteriochlorophyll and a bacteriopheophytin with an ancilliary bacteriochlorophyll molecule has been introduced [AK02b], based on the results of [T8]. Studies of electron transfer (ET) in regular and random protein models have shown that the coupling of the electron to the vibrational dynamics of the protein matrix is vital for the initiation of coherent ET, and allows efficient transfer in the presence of randomness [VHGT, H01, H02b]. Nonlinear charge transport mechanism in periodic and disordered DNA has been analysed. A dynamical approach to protein folding has been studied [TLP]. Further progress has been made in the understanding of the unfolding process in the protein energy landscape in terms of the thermal activation mechanism [BLPT]. A minimal model of polymers has been studied (Kastner & Lazaro), identifying breather solutions under specific topological conditions. In non-homogeneous chains localized chaotic excitations are also expected.

T14 Biomotors The rectification effect via breaking of the friction symmetry [NZCZ-I, NZCZ-II], and through an internal degree of freedom[CFF] was demonstrated. A simple rotator model has been proposed to explain the mechanism of the F_1-ATPase. Theory and experiments on fluxon ratchet motion in Josephson junction arrays have been reviewed[FMMOST]. Soliton ratchet motion via locking of internal mode and the external force was studied[SQ, SZ]. The collective ratchet effect in Frenkel-Kontorova models was characterized[FFMM]. Rectification of particle currents [YFZO, DFL, DKUF], energy currents [FZMF] and spin magnetizations [FMO] due to nonadiabatic nonlinear response to ac fields has been studied in detail. The underlying approach of study and consequent systematic violation of time-space entangled symmetries is of principal importance for the understanding of directed work conducted by biological motors.

T15 Materials Nonlinear wave phenomena, namely modulation instability [CB-I] and solitons [CB-II] in quadratic nonlinear photonic crystals have been studied. The "thermal rectifier" mentioned in Task T5 is also relevant for this task because it uses the nonlinear properties of a model solid material. We investigated the presence of breathers in true materials through the use of molecular dynamics simulation utilizing large scale simulation programs with effective force fields. We have tested the case of long chains hydrocarbons and observed breathers associated with the hydrogen motion. The successful theoretical explanation of localization in PtCl is tantamount to the precise understanding of transport mechanisms in Metal-halogen (MX) materials that can be used in nano-devices. We also began the analysis of a small protein with 56 residues in order to investigate the specific role dynamical localization plays in its function. The aim of this work that is motivated by biomimetics is to attempt a reengineering of systemic parts in the optimized fashion followed by biomolecules.

A.2 Joint Publications and Patents

Throughout the report, young researchers employed on this contract are indicated by an asterisk after their name: Y Zolotaryuk* (Lyngby), G James* (Warwick), A Litvak-Hinenzon* (Warwick), P Maniadis* (Saclay), J Stirling* (Heraklion), F Pignatelli* (Erlangen), A Benabdallah* (Dresden/Lyngby), Matthias Meister* (Zaragoza), Ioana Bena* (Barcelona), JC Comte* (Heraklion), Anna Spanoudaki* (Lyon), T Lazaro* (Firenze), M Kastner* (Firenze), A Vik* (Montpellier).

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A.3 Other publications by YRs

Although not asked for, we think it important also to list any other publications produced or co-authored by the YRs as a result of their employment on the contract.

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A.4 Other publications referred to in this report

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Part B - Comparison with the Joint Programme of Work

B.1 Research objectives

The research objectives set down in Annex I of the contract are still relevant and achievable. Indeed, we have made good progress on all seven objectives: Classical discrete breathers, Quantum discrete breathers in molecular crystals, Vibrational energy distribution and flow, Polarons and bipolarons, Josephson junction arrays, Friction and nonlinear conductivity, and Breathers in biomolecules.

B.2 Research methods

We have followed the research methods specified in the contract, namely, Mathematical proof, Numerical computation, Physical insight, Experiment, and Data analysis.

B.3 Work plan

B.3.1 Breakdown of tasks

Recall that as a result of discussion at the initial network node leaders' meeting in March 2000, we made a few rationalisations to the distribution of the subject matter between the tasks and to their titles, as follows:

T12 We incorporated the protein part of T12 into T13 and the polarobreather part of T12 into T8, and so eliminated T12 as an itemised task.

T3 We added spin systems to T3 and changed the name to "Coupled quantum rotors or spins".

T5 We moved interstellar carbon from T5 to T7, and spectral hole-burning from T5 to T6.

T6 We enlarged the scope of T6 to include temporal randomness as well as spatial.

The tasks and task coordinators are recalled in Table 1.

Task Coordinators		
Task	*Title*	*Coordinator*
T1	Breather existence	Jacques-Alexandre Sepulchre (Nice)
T2	Breather quantisation	Sergej Flach (Dresden)
T3	Coupled quantum rotors or spins	François Fillaux (Thiais)
T4	Breather mobility	Chris Eilbeck (Edinburgh)
T5	Phonon-breather interactions and self-localisation	Thierry Dauxois (Lyon)
T6	Randomness and nonlinearity	Juan Archilla (Sevilla)
T7	Slow relaxation	Roberto Livi (Firenze)
T8	Polarons	Serge Aubry (Saclay)
T9	Josephson arrays	Alexey Ustinov (Erlangen)
T10	Friction and nonlinear conductivity	Claude Baesens (Warwick)
T11	Proton transfer	Mariette Barthes (Montpellier)
T12	Polarobreathers (incorporated into T8 and T13)	
T13	DNA and Proteins	Michel Peyrard (Lyon)
T14	Biomotors	Mario Floría (Zaragoza)
T15	Breather-based materials	George Tsironis (Heraklion)

Table 1: List of tasks and task coordinators.

B.3.2 Schedule and milestones

Tasks

Most of the tasks are on schedule. The only deviations are as follows:

T1 Delay on theory of number of localised modes on a breather. Work not complete on normally hyperbolic persistence theorems and applications.

T2 Rigorous theory of spectral projections not yet totally complete.

T14 Delay in the role of nonlinear localized modes in biomotors.

Milestones

Although we are behind schedule on some of the milestones, we are ahead on others, so overall the situation looks good.

6-month milestones: All done, except for submission of an essentially complete paper on existence of globally attracting sliding state for overdamped tilted FK models (Baesens & MacKay).

12-month milestones: We have not yet developed the proposed data analysis techniques for extracting spatial correlation lengths of vibrations from neutron scattering experiments, but have prepared a plan, and it is a question of finding a suitable postdoc. For the number of local modes on a breather, the DNLS case is clear, and work of Kim suggests how to tackle the general case but we have not yet exploited it. The groundwork for understanding generalised multibreathers in dissipative oscillator networks has been done already by Bates in a different context, so we will adapt this, but conceptually there is little more to do.

18-month milestones: We have assessed the role of breathers in interstellar carbon [KA01] and spectral hole-burning, and are making progress on their role in 4-methyl pyridine, DNA and some biomotors. We have formulated a theory of quantum breathers as spectral projections [M2]: just the finishing touches remain to make it rigorous.

24-month milestones: We have already made some progress on the theory of breather mobility in 1D [MS02], but interesting new observations of Eilbeck in 2D present challenges on this topic which we aim to address shortly.

30-month milestones: We already made some progress on the role of DB in heat conduction (T10) and Hydrogen-bonded systems (T11).

36-month milestones: We already made progress in CDW conductivity (Baesens, Floria, MacKay & Sancho), proton transfer (see T11 report), and thermal relaxation (see T7 report).

B.3.3 Research effort

The research effort during the period is summarised in Table 2.

B.4 Organisation and Management

B.4.1 Description

The management has continued to be a combination of hierarchical (via the tree in Table 3 of the contract) and horizontal (via task coordinators). Virtually all communication is via e-mail. Information is disseminated via the webpage http://www.maths.warwick.ac.uk/~mackay/locnet.html for the network. This includes links to webpages for most of the nodes, network meetings, network vacancies, the network's publication archive http://www.ma.hw.ac.uk/LOCNET/publications.html and the Cordis database.

A notable development is the establishment of formal links between the network and the USA. Sievers (Cornell) and Tsironis (Heraklion) obtained an NSF grant to enable USA researchers to participate in a joint meeting with LOCNET in Crete in June 01; it seems we were chosen by the NSF as a test case for the possibility of more extensive NSF funding of collaboration with EC networks, and the initiation of American networks. Sievers also obtained NSF money to send 4 graduate students at USA universities to LOCNET nodes for summer projects in 2002.

Professional Research Effort Spent on the Network Project					
Participant	*Subcontractor*	*Associate*	*YRM*	*ORM*	*NR*
1. Warwick			12	23.5	9
	Edinburgh		0	8	4
		Cambridge	0	15	4
2. Saclay			12	40	5
	Lyon		3.5	20	7
		Nice	0	3	1
3. Erlangen			12	30.5	4
	Dresden		12	43	6
		Berlin	0	3	1
4. Zaragoza			4.8	32	6
	Barcelona		1.4	6	2
	Madrid		0	3	2
		Sevilla	0	10	5
5. Lyngby			12	17.5	7
6. Heraklion			6	60	5
	Athens		0	3	1
7. Firenze			10	13	5
		Salerno	0	8	2
		Milano	0	2	1
8. Thiais			0	12	1
		Montpellier	8	6	3
TOTALS			87.7	362.5	83

Table 2: Number of person-months of professional research effort by participant spent on the project during the reporting period, including the indicated dependent subcontractors and associates, differentiating between young researcher months (YRM) financed by the network and other researcher months (ORM) financed from other sources (including the group leaders), and indicating the total number of researchers who contributed to the project (NR).

Furthermore, the network organised a minisymposium on "Localisation and energy transfer in spatially discrete systems" at the SIAM conference on Applications of Dynamical Systems in Snowbird USA in May 01, and Flach (Dresden) and Bishop (Los Alamos) organised a month-long event in Dresden in Sept 01, with several USA participants (despite September 11).

We are expecting a number of people from outside our network at our forthcoming network meeting at El Escorial in June 02, and several LOCNET members have been invited to a meeting at Los Alamos in July 02 on "Intrinsic localized modes". LOCNET members form an important part of a Euroconference proposal on Localization, headed by Bountis (Patras) and involving several people from the USA. Sievers is planning a NATO-funded Erice meeting. Also worth mentioning is that LOCNET has combined forces with a Mathematics EC RTNetwork called MASIE to propose a series of PhD Euroconferences on Dynamics, Mechanics and Symmetry (coordinator: Claudia Wulff).

B.4.2 Network Meetings

Nonlinear Science Festival III, 12-15 June 2001, Lyngby Although not an official network meeting, Bang (Lyngby) was one of the main organisers and a number of people from the network participated: Scott, Bang, Aubry, Stirling*, including a talk by Stirling*.

Node leaders' meeting, Heraklion, 13 June 2001 Aubry, MacKay, Fillaux, Archilla, Ustinov, Eilbeck, Tsironis, Barthes, Sancho, Floria, Hennig (+ Flach, Sepulchre?). Also, Gaididei represented Christiansen, and Sievers (Cornell) attended to present his plans for further USA links with LOCNET. We planned future events, notably El Escorial 17-21 June 02 and the mid-term review Warwick 23-24 Sept 02. We identified the tasks needing attention and assigned responsibility for carrying them forward. We discussed YR recruitment problems and planned contingency measures should these not be resolved; in the event these have not been necessary.

EU-US meeting on Discrete Breathers, 13-16 June 2001, Heraklion This meeting, organized by A Sievers and G Tsironis, was a major event since it brought basically all the world experts on breathers to Crete for exchange and discussions. The American scientists were funded directly by NSF who provided a grant especially for this meeting. LOCNET speakers: Archilla, Aubry, Barthes, Benabdallah*, Dorignac, Eilbeck, Eleftheriou, Fillaux, Fistul, Flach, Floria, Gaididei, Henning, James*, Kadelburg, Kopidakis, MacKay, Maniadis*, Miroschnichenko, Pignatelli*, Sancho, Schuster, Tsironis, Y.Zolotaryuk*; additional LOCNET participants: Catarino, Litvak-Hinenzon*, Mazo, Morgante, Piazza, Ustinov, Voulgarakis.

Special session in "4th discussion meeting on relaxations in complex systems" , organized by G Tsironis (Hersonisos, Crete 17-25 June, 2001). The Heraklion node was invited to organize a special session in the very large (approx 800 participants) "4th discussion meeting on relaxations in complex systems", focusing on breathers and their connection to glasses and biomolecules. In this session interaction took place between LOCNET members and scientists from USA and Japan as well as from other scientific areas. LOCNET speakers: Aubry, Flach, Tsironis

Nonlinear Lattice Structure and Dynamics, Dresden, 3-28 Sept 2001 organisers: Flach (Dresden), Bishop (Los Alamos). The event was divided into 4 weeks, consisting of 3 focus weeks on the following topics: nonlinear deformation waves, computational approaches to nonlinear phenomena in discrete systems, quantization of localized excitations on lattices, and concluding with a workshop on localized excitations on lattices. LOCNET participants: Aubry, Bambusi, Benabdallah*, Dorignac, Eilbeck, Eleftheriou, Fillaux, Fistul, Flach, Floria, Gaididei, Henning, Kadelburg, Kopidakis, Leon, Lepri, Mingaleev, Miroshnichenko, Morgante, Pignatelli*, Salerno, Sepulchre, Theodorakopoulos, Tsironis, Ustinov, Vik*, Voulgarakis, Y.Zolotaryuk*, Sanchez-Rey, Cuevas, Palmero, including talks by YRs Benadbdallah*, Pignatelli* and Zolotaryuk*.

Mathematical Interdisciplinary Research day on Discrete Breathers, Warwick, 29 Nov 01 organised by Litvak-Hinenzon* (Warwick); LOCNET speakers: Fillaux, Sepulchre, James*, Flach, Floria

B.4.3 Other Networking

Individual visits between nodes

- Peyrard (Lyon) to Lyngby (1-10 March 01)
- Theodorakopoulos (Athens) to Lyon (12 – 17 March 2001)
- Salerno (Salerno) visited Sevilla (19-22 March 2001).
- Stirling* (Heraklion) to Lyngby (18 Apr - 2 May 01 and 10-17 June 01).
- Ibañes (Barcelona) to Heraklion 20 - 26 May 2001.
- Lazaro* and Kastner* (Florence) visited Bambusi in Milan.
- Schjeodt-Eriksen (Lyngby) to Lyon (1 May – 15 July 2001).
- Archilla (Sevilla) to Lyngby (22 Oct - 22 Dec 01).
- Zolotaryuk* (Lyngby) to Dresden (1-12 Apr 01).
- Zolotaryuk* (Lyngby) to Salerno (18 Apr - 3 May 01).
- Tsironis (Heraklion) to Barcelona 4-8 April, 29 July - 17 August and 18-21 Dec 2001.
- Zolotaryuk* (Lyngby) to Dresden (3-28 Sep 01).
- Floría (Zaragoza) to Barcelona, 3 - 4 and 14-16 October 2001.

- Pignatelli* (Erlangen) visited Zaragoza (5 Nov 01).
- Floría (Zaragoza) visited Warwick (One month, Nov 01).
- I.C. Bena* (Barcelona) to Zaragoza 21 - 23 January 2002.
- Floría (Zaragoza) visited Dresden (3 weeks, Feb 02).
- Archilla visited Berlin (22 January - 3 March 2002).
- Archilla visited Erlangen one day (4 May 2001).
- Stirling* (Heraklion) visited Barcelona and Zaragoza (7-14 May 01) and obtained two job offers. He accepted a job at the University of Barcelona.
- Elefteriou and Voulgarakis (Heraklion) visited Dresden for collaboration and workshop participation.
- Fistul (Dresden) visited Erlangen and gave a talk at the seminar on December 12, 2001.
- Jerome Leon (Montpellier) visited Erlangen and gave a talk on February 7, 2002.

Visits by YRs to other workshops and conferences

- Y. Zolotaryuk* (Lyngby) visited the annual meeting of the German Physical Society on Condensed Matter Physics in Hamburg (26-30 Mar 01).
- Y. Zolotaryuk* (Lyngby) participated in the conference "Physics of Information and Synchronization in Stochastic Dynamics", Dresden (1-4 Apr 01) and presented a poster with the title "Symmetry approach to rectification of currents in ac-driven nonlinear systems".
- probably many others

E-discussion

JC Comte* (Heraklion) has been using Net-meeting with France on a regular basis for collaborative work. It has proved to be quite useful.

Approved non-EU travel

Dauxois and MacKay were approved travel to Snowbird, USA, to present the work of the network at the SIAM Applications of Dynamical Systems conference, May 2001.

B.5 Training

B.5.1 Advertisement of vacant positions

Advertisement this year has been as follows:

Lyon: Cordis site, personal website, personal contacts, e-mail

Zaragoza: Internet forum Fisica Estadistica, locnet website

Warwick: www.jobs.ac.uk, Maths dept webpage, locnet webpage, Cordis site

Edinburgh: locnet webpage, Cordis site

Firenze: INFM web-page, tip-top, colleagues around the world, locnet webpage

Heraklion: We advertised through the network web page and by sending individual email messages to selected researchers around the world working in similar areas and who have students.

Athens: YR position advertised (beyond collective Physics Today & Locnet node), in the web (TIPTOP, CORDIS, locnet website, own inst. website), email to colleagues.

Barcelona: Web (http://www.tp.umu.se/TIPTOP and http://physicsweb.org).

Montpellier: Cordis, locnet website

Thiais: Cordis, locnet website

B.5.2 Progress in recruitment

The YR months financed by the contract so far are indicated in Table 3. Commitments to existing and recently selected YRs are Saclay (+Lyon): 9.5 (+8.5), Warwick: 11.2, Erlangen: 17.5, Lyngby: 20.6, Firenze: 26, Zaragoza (+Barcelona): 24.2 (+10.6), Heraklion (+Athens): 6 (+10). Some extensions of and further appointments are expected in the near future.

Young Researcher months financed by the contract						
	Contract deliverable			*YR months financed so far*		
Participant	*Predocs*	*Postdocs*	*Total*	*Predocs*	*Postdocs*	*Total*
1. Warwick, UK	0	50	50	0	21.7	21.7
2. Saclay, FR	0	42	42	0	16	16
3. Erlangen, DE	36	8	44	18.5	18	36.5
4. Zaragoza, ES	0	40	40	0	6.2	6.2
5. Lyngby, DK	0	35	35	0	14.4	14.4
6. Heraklion, GR	0	38	38	0	12	12
7. Firenze, IT	0	58	58	0	10	10
8. Thiais, FR	0	22	22	0	8	8
TOTALS	36	293	329	18.5	106.3	124.8

Table 3: Numbers of young researcher months financed by the contract and numbers used by 28 February 2002.

B.5.3 Integration of young researchers

All the nodes with YRs have integrated them actively into their research environment. In addition: M. Meister* (Zaragoza) is actively cooperating in the supervision of an undergraduate (last year) student who was awarded a grant of Initiation to Research by the University of Zaragoza; A. Litvak-Hinenzon* (Warwick) organised Breather group meetings at Warwick, with both internal and external speakers, and a one-day meeting with international speakers.

B.5.4 Special training measures

Francesca Pignatelli* (Erlangen) learned to measure in a temperature-controlled environment using a ^{4}He cryostat.

B.5.5 Equal opportunity measures

We have been open to applications by women, and 5 of the 14 YRs appointed so far are women. We have made a conscious effort to give women positions of responsibility in the network, e.g. one of the node leaders and two of the task coordinators.

B.5.6 Multidisciplinary training measures

The YRs of the Florence node profited greatly from a special school organized by some Locnet members for training physicists, mathematicians and engineers in molecular biology at a basic level. The school entitled "The basis of molecular biology" was held at the University of Florence from 12 - 14 February 2002.

In the group meetings at Heraklion, Comte* has been introduced to multidisciplinary topics, in particular connections of physics with biology.

B.5.7 Industrial and commercial training

None this year.

B.6 Difficulties

A major administrative difficulty occured for the appointment of a post-doc, Jens Schjoedt-Eriksen, by CEA Saclay. The first request to CEA was made in February 2001 by M. Peyrard (Lyon), with a view to a start date of 1 May. But the paperwork was not ready by that date, so J. Schjoedt-Eriksen had to start as a visitor rather than a postdoc. By July the hiring had still not been completed, nor even formally confirmed, and in the meantime the applicant accepted another job offer which looked more secure.

Work on mobile breathers has been delayed by setbacks in hiring a YR at Heriot-Watt. Two potential candidates are however under consideration now.

The position at Athens has been difficult to fill: it was offered to 3 suitable candidates who each chose jobs elsewhere. But an appointment has just been made.

The coordinator (MacKay) had two other major administrative responsibilities this year (assessor of UK research in Applied Mathematics, and organisation of a large UK Mathematics conference) so has not been able to put much time into the research, but hopes the situation will now return to normal. Baesens (Warwick) has been on sick/maternity leave since 3 Aug 2001, but is expected to return to work on 25 May 2002.