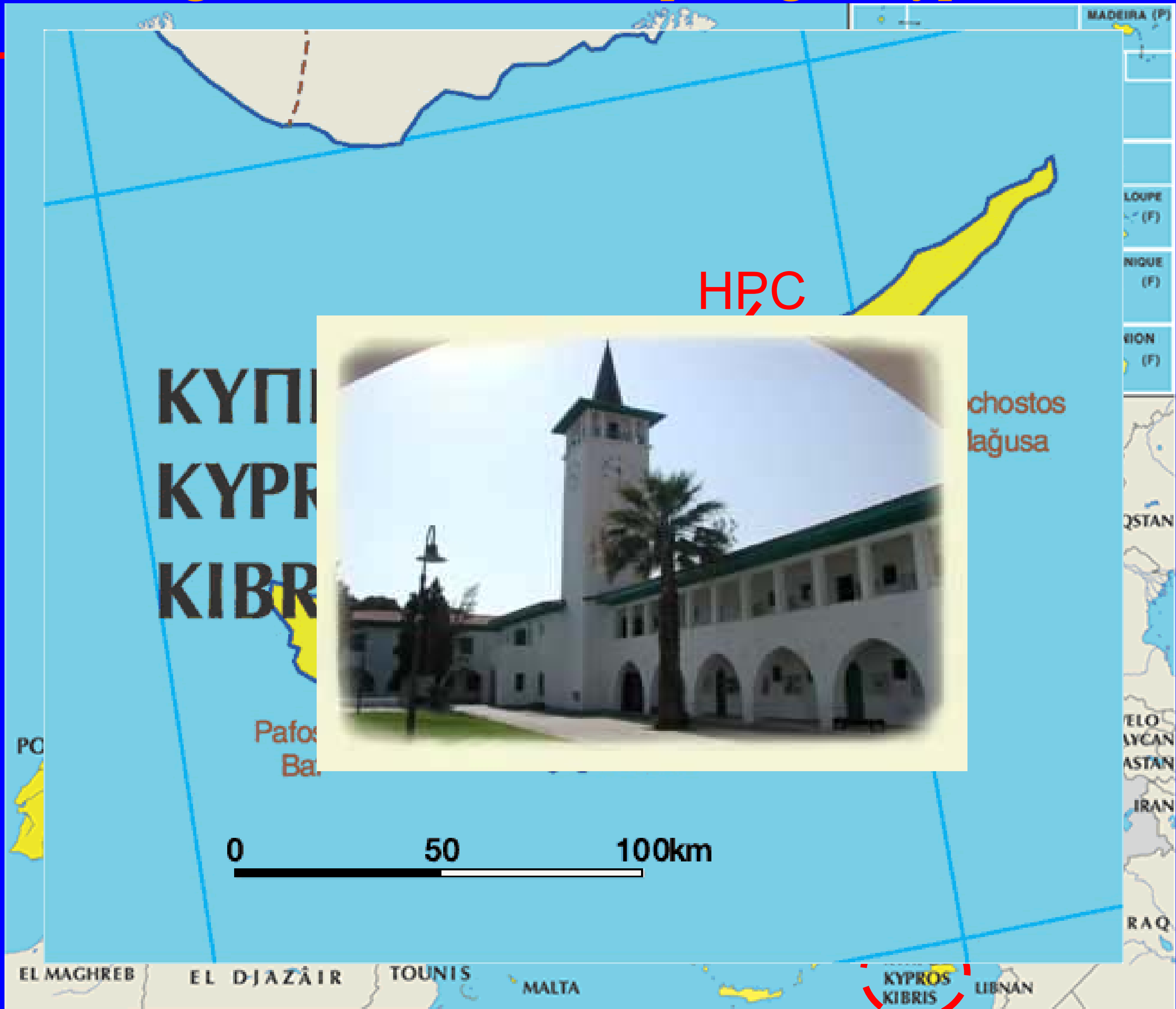
High Performance Computing in Cyprus



Facilities

• **University of Cyprus:**

No central facility exists. Only smaller units that belong to various research groups

→ **large scale applications must be run outside Cyprus**

Yearly Budgetary constrains allow the purchase of only small scale clusters

↪ **Big Problem!!**

• **Frederick Institute of Technology (Private College):**

64 - node Opteron cluster, bought for Lattice QCD calculations (C. Strouthos)

HPC at the University of Cyprus

http://www.ucy.ac.cy/facultiesE/facultiese.html

- **School of Pure and Applied Science:**

  - **Department of Physics (Total of 190 processors):**
    - Theoretical Biophysics → 2 faculty
    - Lattice Quantum Chromodynamics (LQCD) → 2 faculty
    - Experimental Nuclear Physics → 1 faculty
    - Experimental High Energy Physics → 2 faculty
  - **Department of Computer Science:**
    - GRID applications
  - **Department of Chemistry (no cluster facilities):**
    - Materials Chemistry, Quantum Chemistry applications
  - **Department of Mathematics and Statistics (no cluster facilities):**
    - Fluid dynamics, Oceanography
  - **Department of Biology (no cluster facilities):**
    - Bioinformatics

- **School of Engineering (Talk by Stavros Kassinos)**

- **School of Economics and Management:**
  - **HERMES European Center of Excellence on Computational Finance and Economics**

Computational Finance and Economics

HERMES Center established the first high-performance parallel computing laboratory in Cyprus in 1993 purchasing a 4x4 RISC processor Parsytec computer and gaining the status of European Center of Excellence in 2002

Research Area:

Development of innovative models for managing international portfolios, for corporate bond portfolios and for computer-aided design of financial products

Important studies:

1. **Pioneered a major international study on the structure of household portfolios in collaboration with research centers in Italy, the Netherlands and the Federal Reserve in the US**
2. **A Pan-European Study on the performance of financial institutions developed a major database for use by researchers studying drivers of performance of financial institutions in collaboration with the Wharton Financial Institutions Center in the US**

➡ **Promoted the establishment of the Real Option Group, an international organization promoting research and training in the field of finance**

However 1996 Parsytec Parallel Computer not upgraded

Department of Physics

Theoretical and Computational Biophysics

Computational resources: Linux clusters

Heracles

1 master + 16x2 3.0-3.2 GHz Intel Pentiumm nodes

Fast Ethernet internode communication

Odysseas

1 master + 12x2 2.4 GHz nodes

Myrinet internode communication

Yearly Budgetary limits only permit the purchase of small scale clusters at a time

Software:

MD, MC, Continuum Electrostatics:

- ***CHARMM (version c32*)***
- ***AMBER7***
- ***INSIGHT (linux version)***
- ***BOSS 4.2***
- ***UHBD 5.1/MEAD***

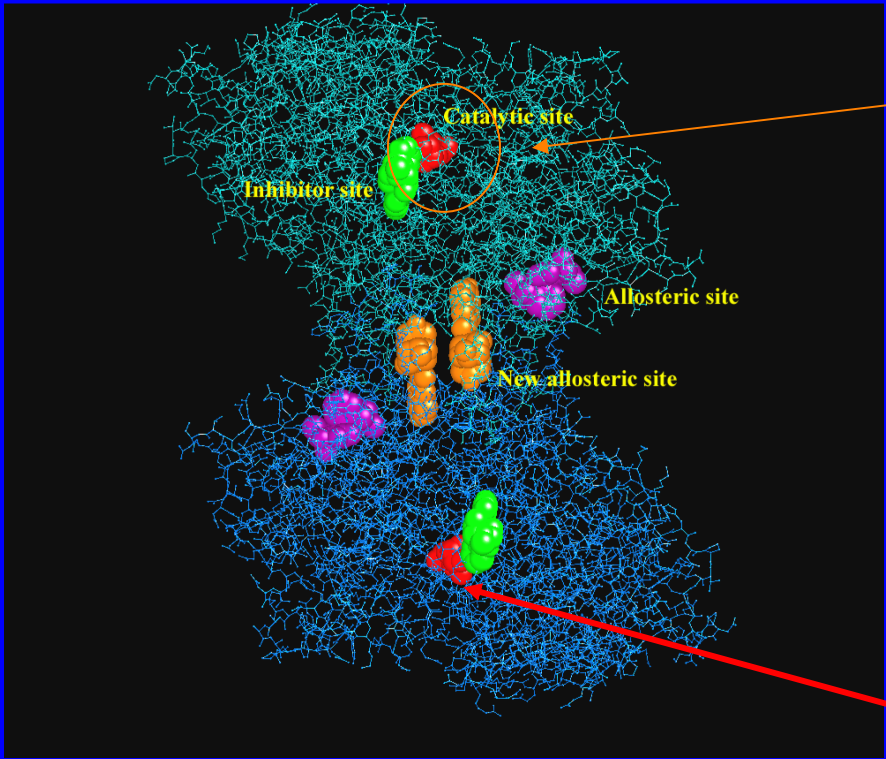
QM / electronic structure:

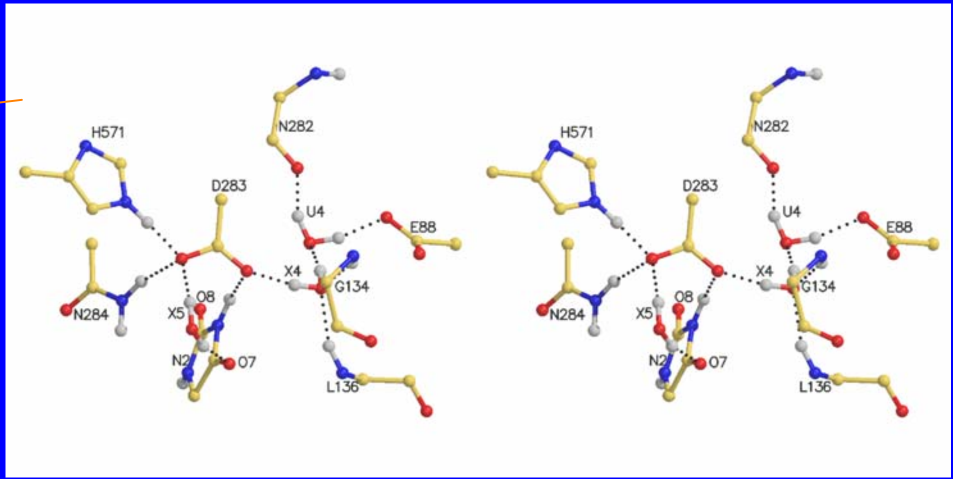
- ***Gaussian 98/03***

Thanks: G. Archontis and S. Skourtis
Department of Physics
http://www.biophys.ucy.ac.cy

Biophysics Applications

- Glycogen Phosphorylase (~20,000 atoms)





Catalytic site interactions

Molecules external to the protein interacting with it. Interactions modeled on an atomic level

10^8 MD steps: Multi-ns MD simulations done on a 32-processor cluster
Free-Energy transformations can be run as concurrent simulations in different nodes => trivially parallelizable problem.

Biophysics Applications

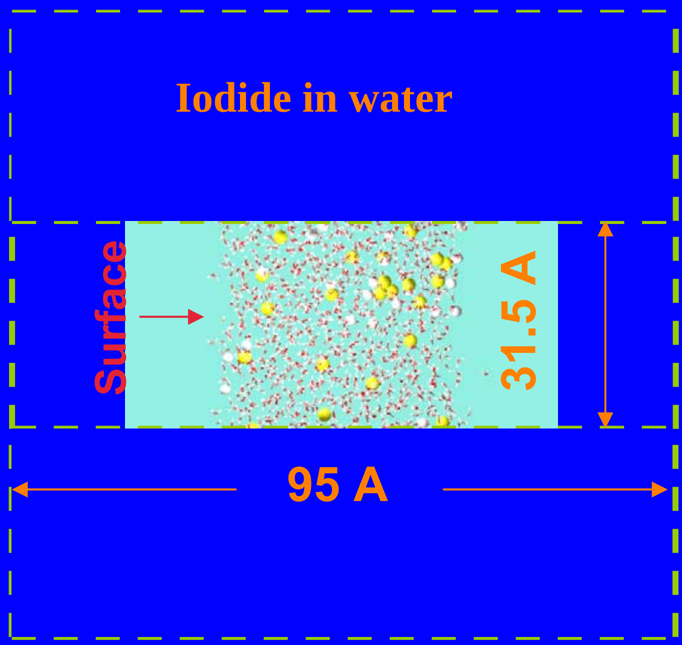
- **Directed Evolution Simulations of Protein Design: fix protein structure and change chemical type and orientation of constituent monomers → minimize energy**

Typical Protein Design Simulations: 10^9-10^{12} energy evaluations over protein sequences / sidechain rotamer states.

Each processor handles changes at a subset of the positions → trivially parallelizable problem => more processors will allow for larger number of sequence/fold exploration.

G. Archontis and T. Simonson, J. Phys. Chem. B 109:22667(2005)

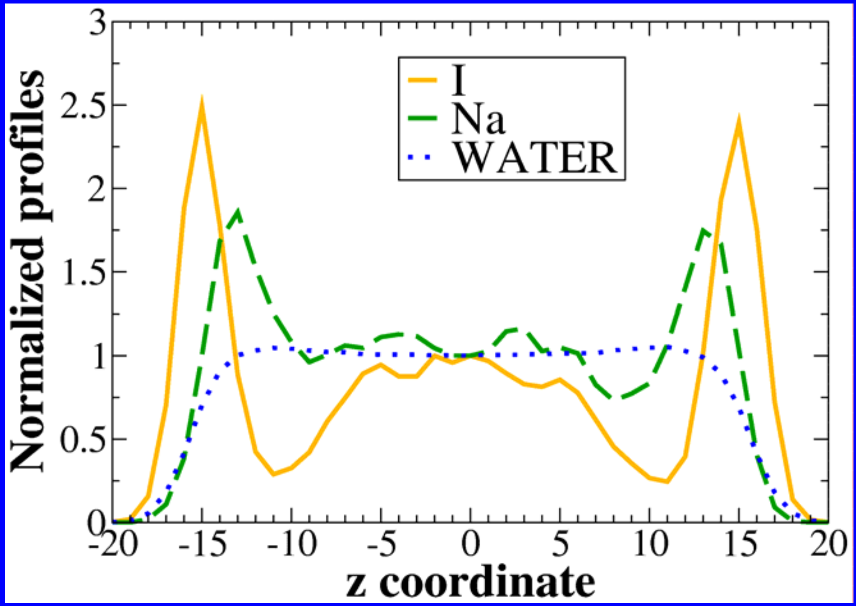
- **Ion solvation at the air-water interface**



▶ A most important model system, since no interactions exist with the second (gas) phase, and the interface acts only as a discontinuity for all interactions, creating a significant asymmetry

Chaotropic ions: destabilize structure of water e.g. I

Cosmotropic ions: stabilize the H-bonding structure of water e.g. F^-



- **MD simulations with a new polarizable model for water/ions prove that large chaotropic ions prefer interfacial solvation sites**

- **Cavity formation interactions favor the interfacial position. Interactions between permanent charges (Onsager model) favor the bulk. Interactions related to induced charges stabilize the interfacial location**

Archontis et al., J.Phys.Chem. B 109:19757 (2005)

The MD simulations were run in small systems (1000 water molecules with 22 ions of each sort, typical of NaCl concentrations in seawater), and for rather short times (2-4 ns). Still simulations needed for convergence require order of months on a 16-node, 3 GHz/node cluster :

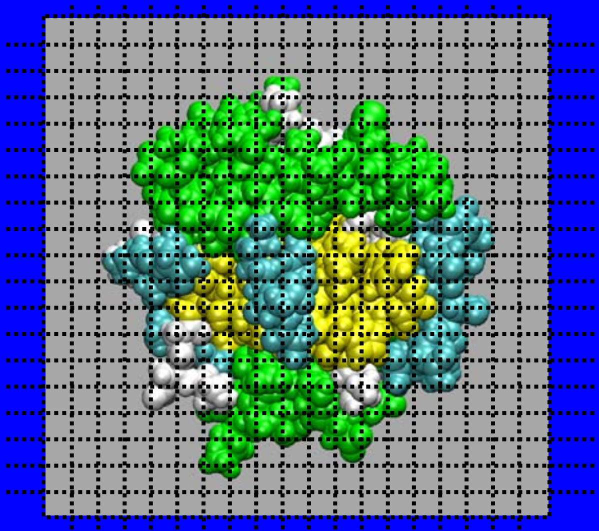
- Equilibration is not perfect (asymmetry in graph, pair correlation function should go to unity in the middle of the water slab)

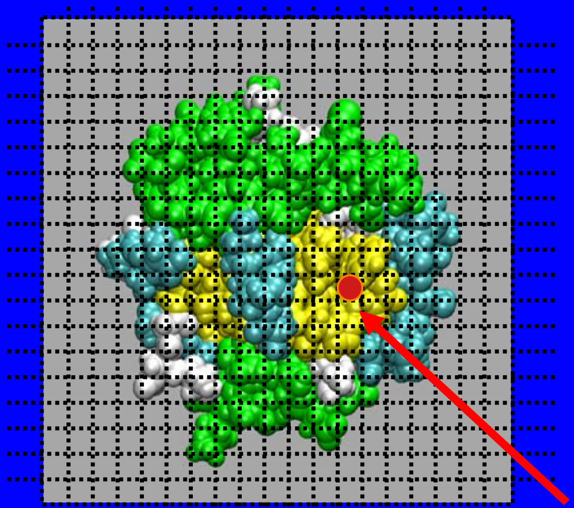
- To check the validity of the results one needs to run the simulations in larger systems (one order of magnitude) and for much longer times

Access to supercomputers necessary

Biophysics Applications

- Calculation of Proton Binding with MD and continuum Electrostatics





- Multi-ns MD simulations of protein+explicit water => structure generation.
- Solution of the Poisson-Boltzmann equation for 10^3 structures of each state.

G. Archontis and T. Simonson, Biophys. J 88 3888 (2005).

- Electron transfer theory and computation
  - ➢ Computation of dynamical effects on biological electron transfer rates
  - ➢ Computation of tunnelling matrix elements for biological electron transfer systems
  - ➢ Development of theory/methodology for electron transfer through fluctuating molecular media

Electron transfer computational projects

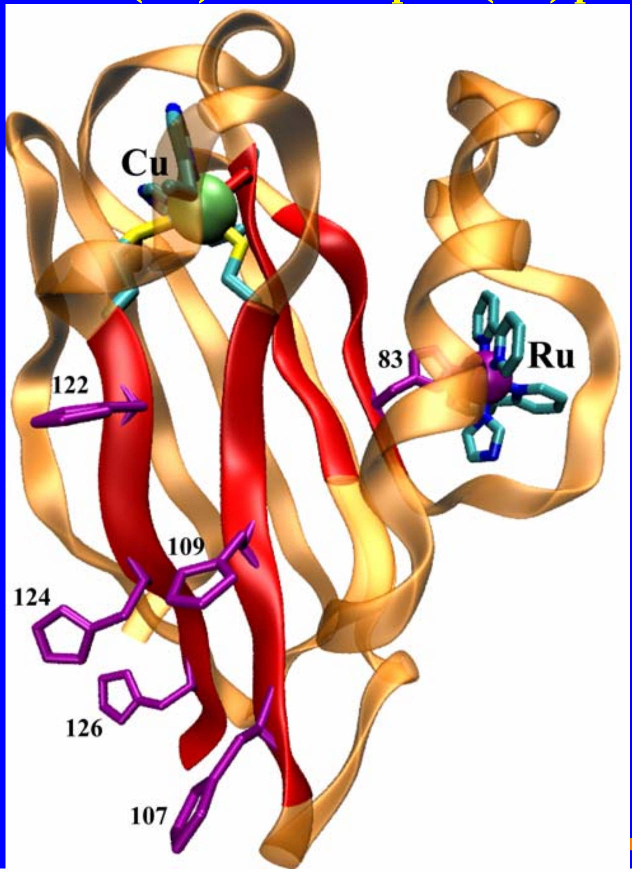
• **Electron transfer in Azurin**

- MD simulations for structure production, 18,300 atoms total (Duke U. CSEM cluster, 300 processors)

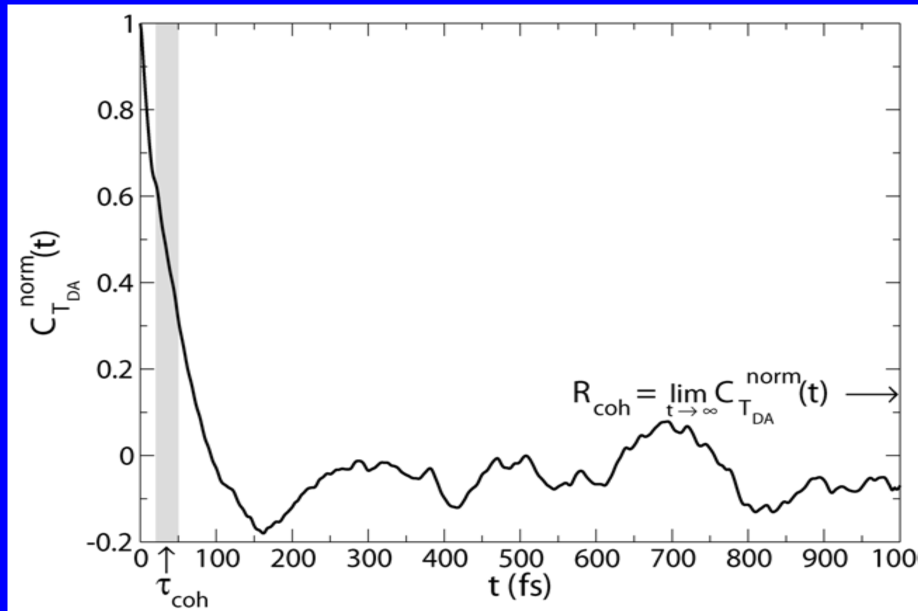
- Constrained MD simulations/semi-empirical tunneling matrix element calculations (University of Cyprus clusters)

Dynamical effects on electron transfer rates in azurin

Protein structure showing electron donor (Cu) and acceptor (Ru) positions



Donor-acceptor tunnelling matrix element correlation function showing coherence time



S. Skourtis, et al. Proc. Natl. Acad. Sci. (USA) 102 (2004)

A. Teklos and S. Skourtis, Chem. Phy. 319 (2005)

Electron transfer computational projects

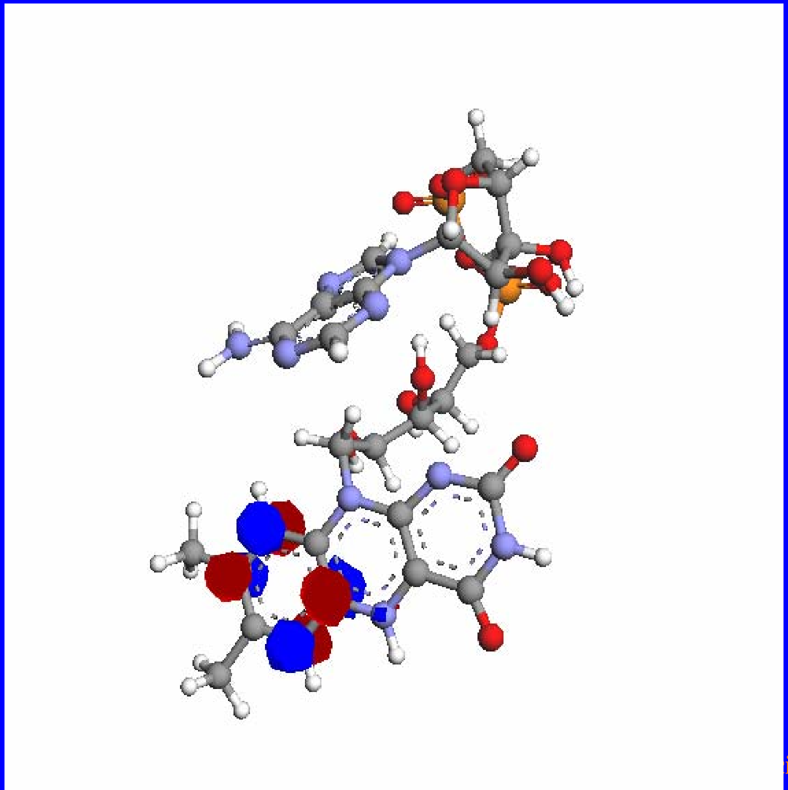
- **Photoinduced electron transfer in DNA-Photolyase (protein responsible for fixing DNA damage)**

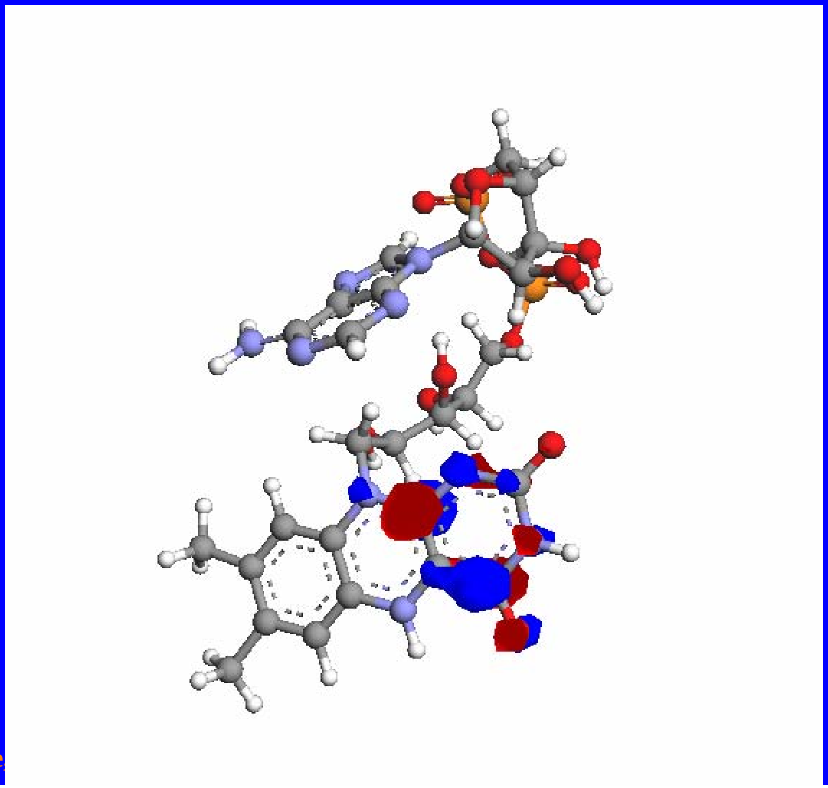
  - Computation of photoexcited electron donor states and tunneling matrix elements with electron acceptor (University of Cyprus clusters)

  - Ab-initio and semi-empirical electronic structure methods: ZINDO, CIS, TDDFT

Photoinduced electron donor singlet states in the active site of DNA-Photolyase

$FADH^-$ cofactor





Future plans & needs in Biophysics

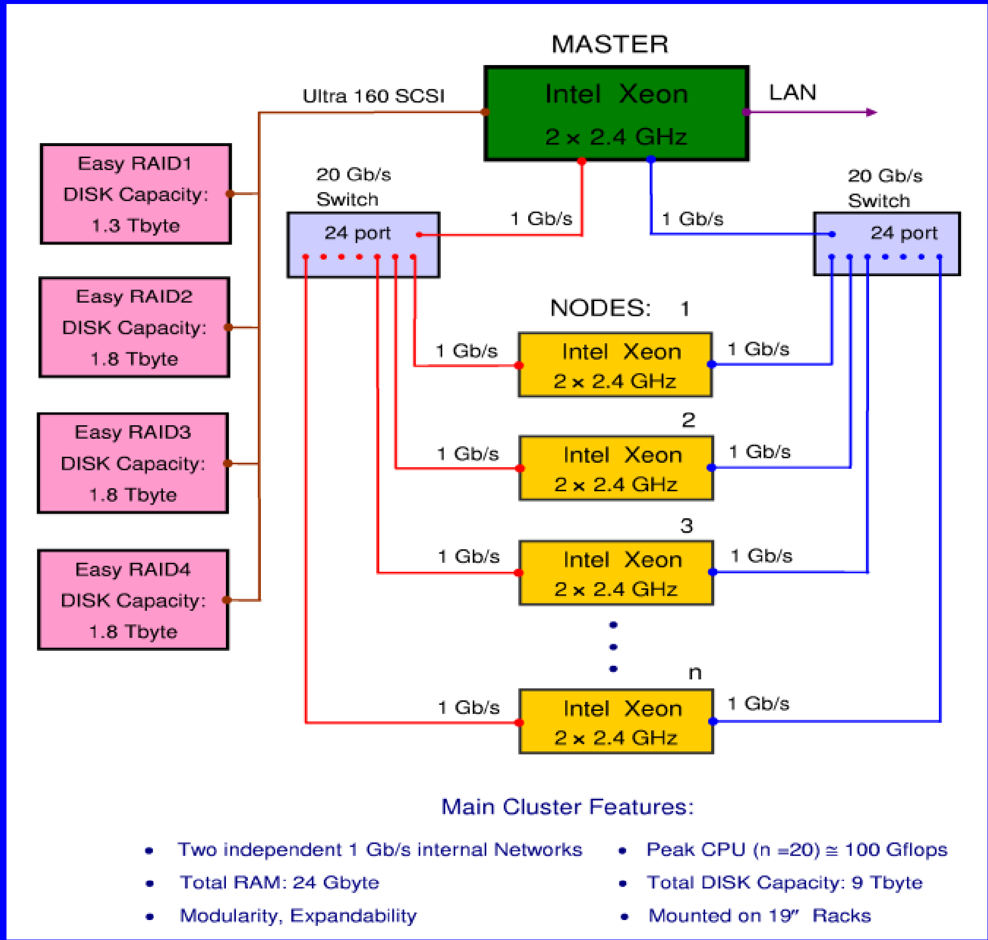
- **Methods**
  - Ab-initio MD simulations.
  - Ab-initio nonadiabatic MD simulations.
  - QM/MM simulations.
  - Protein design simulations, applied to entire protein families.

- **Needs**
  - Access to large numbers of processors
  - (Truly parallel and trivially parallel calculations)

Experimental Nuclear and Particle Physics

Two clusters:

- ➔ 25 + 10 dual nodes (2.4 GHz)
- ➔ 10 Tbyte disk storage



Linux cluster

Software: Pluto, Hydra, UrQMD, Hgeant, Oracle Interface

Thanks H. Tsertos
Department of Physics

Applications

• **HADES experiment at GSI with beam energies of 4.5 GeV protons and 1-2 AGeV heavy ions:**

- **The study of electron-positron pair emission in relativistic heavy-ion collisions**
- **Di-lepton production in elementary reactions and experiments aimed at studying the structure of hadrons.**
- **The study of vector meson mass distributions.**
- **The study of chiral symmetry restoration to elementary properties of hadrons.**

• **Compressed Baryonic Matter (CBM) experiment at GSI:**

- **The study of in-medium properties of hadrons**
- **The search for the chiral and deconfinement phase transition at high baryon densities**
- **The study of the nuclear equation of state of baryonic matter at high densities**
- **The search for the critical point strongly interacting matter**
- **The search for new states of matter at highest baryon densities**

• **CMS experiment at CERN:**

- **Electromagnetic Calorimeter**
- **Analysis and Software**

Lattice QCD

Again purchased in units of 8 nodes yearly due to budget constrains

Enough for the group for small projects.

Larger scale must be run on machines outside Cyprus e.g. NERSC, NIC

Many thanks to Th. Lippert and N. Attig for their support in using JUMP at NIC

Two 8-dual nodes connected with Gb´s ethernet

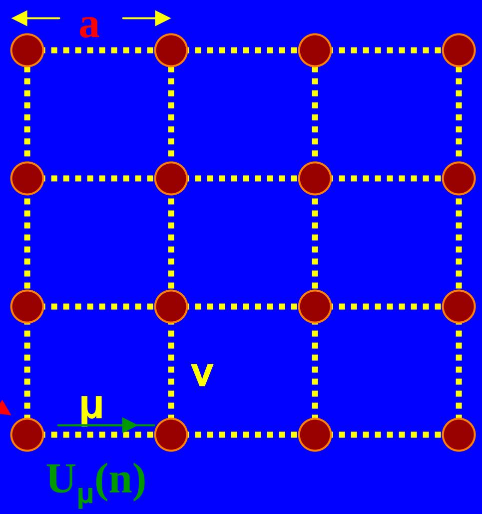
Two 8-dual nodes connected with Myrinet

- 64 processors with the newest 3.6GHz

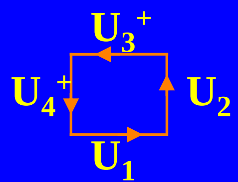
Lattice Quantum Chromodynamics

Gauge theories on the lattice: The simplest discretisation of the 4-dimensional Euclidean space is to use an isotropic hypercubic grid with the same lattice spacing in all directions.

Symmetries: Gauge invariance is preserved exactly



Fermion fields are defined on sites: ψ(n)

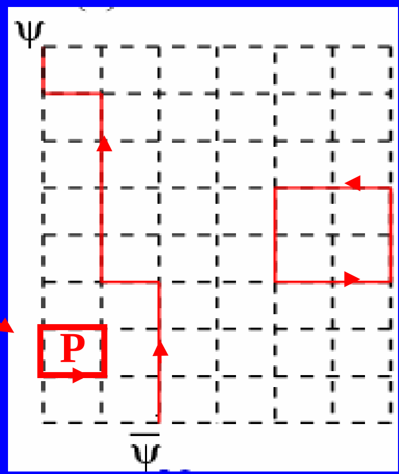


$U_P = U_1\, U_2\, U_3^+\, U_4^+$

$e^{igaA\mu(n)}$

gauge invariant quantities

smallest possible



$\sum \left(\quad \right) \rightarrow 1/4 F^a_{\mu\nu} F^{a\mu\nu}$

Observables in LQCD

Physical results are extracted by calculating expectation values like in Statistical Mechanics:

$$\hat{\ } \quad \frac{\int \mathbf{D} \quad \mathbf{D} \; \mathbf{D}}{\int \mathbf{D} \quad \mathbf{D} \; \mathbf{D}}$$

→ Integrating out the Grassmann variables is possible

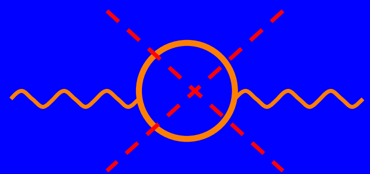
$$\hat{\ } \quad \frac{\int \mathbf{D} \quad \{ \quad \}}{\int \mathbf{D} \quad \{ \quad \}}$$

3x3 Unitary matrix:

16^3x32 lattice: ~10^7 degrees of freedom

Sparse matrix of dimension ~10^7

Quenched approximation: set det D=1



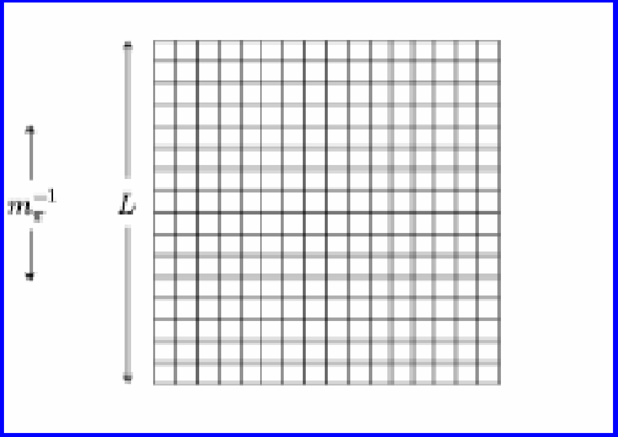
omit pair creation

→ Easy to simulate since S_g[U] is local: use M. C. methods from Statistical Mechanics like the Metropolis algorithm ➡ can be done carried out on our cluster

$$\hat{\ } \quad — \quad \sum_{\in \frac{1}{Z}}$$

1. Generate a sample of N independent gauge fields U
2. Calculate propagator D^{-1} for each U

Computational aspects



- Fermion determinant – Full QCD
- Lattice spacing a small enough to have continuum physics
- Quark mass small to reproduce the physical pion mass
- Lattice size large enough so that $\leq 4 -$

L (fm)	m_π (MeV)
1.6	560
2.5	360
4.5	200
6.4	140

most quenched calculations reaching ~400 MeV pions

Computational cost ~ $(m_q)^{-4.5}$ ~ $(m_\pi)^{-9}$

Currently we are starting to do full QCD by including the fermionic determinant but we are still limited to rather heavy pions → understand dependence on quark mass

Physical results required terascale machines

Applications

• **Small projects run on Cyprus cluster:**

- **16^3x32 lattices for pentaquark project,** *C. Alexandrou and A. Tsapalis, PRD (2006)*
- **16^3x32 and 20^3x32 lattices for probing diquark dynamics,** *C. Alexandrou, Ph. de Forcrand and L. Biagio, Lattice 2005*
- **Calculation of static multiquark potentials,** *C. Alexandrou and G. Koutsou PRD 71(2005)*
- **Perturbative lattice calculations up to three-loops (e.g plaquette with Clover fermions),** *H. Panagopoulos et al., hep-lat/0601009*
- **Simulations of large SU(N): topological charge and susceptibility,string tensions for different representation of SU(N), glueball masses and their dependence on the topological sector,** *L. Del Debbio, H. Panagopoulos and E. Vicari, Lattice 2005*
- **Hadron density-density correlators wave functions,** *C.Alexandrou et al.. Lattice 2005*

training of students and, to a less degree, postdocs

Applications

• **Larger projects run on NIC and NERSC:**

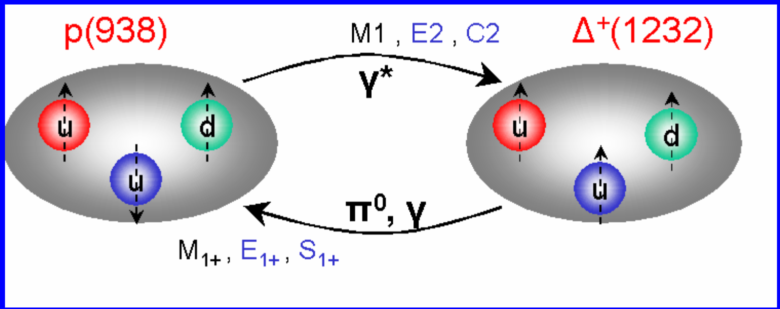
➢**Electromagnetic properties:**

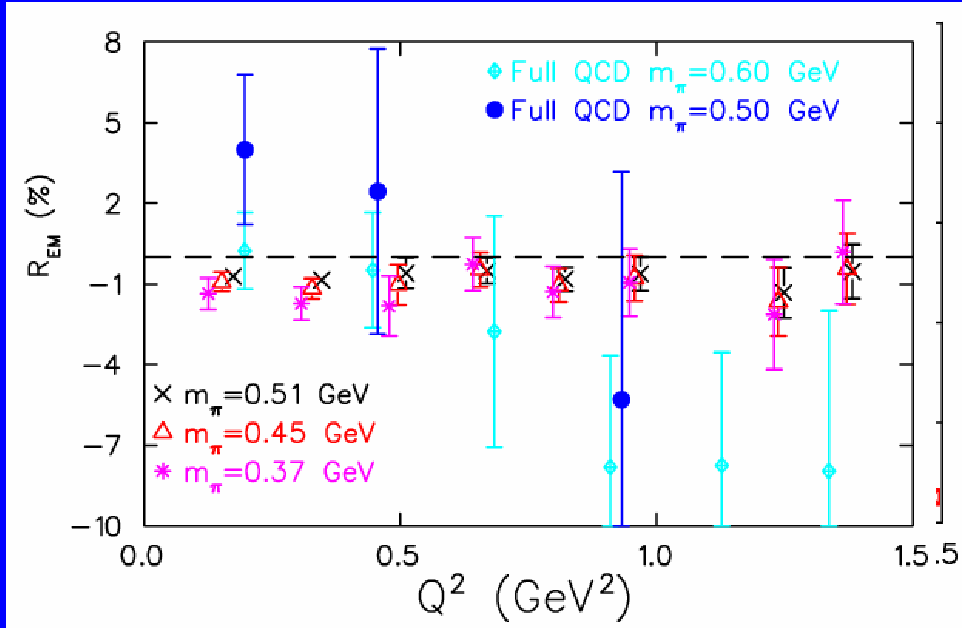
- γN→ Δ using chiral fermions on the MILC dynamical configurations, ***C. Alexandrou et al. PRL94 (2005)***

- nucleon elastic form factors using dynamical Wilson fermions obtained from the group of K. Jansen

➢ **Hadron wave functions via density-density correlators**

➢**Axial N to Δ transition in quenched QCD on a 32^3x64**





Three transition form factors, Γ_{M1}, Γ_{E2} and Γ_{C2}

→ non-zero E2 and C2 multipoles signal deformation

Department of Computer Science

Grid in Cyprus

- **Activities:**
  - –Established and operates a Cypriot Grid infrastructure connected to international Grid testbeds.
  - –Established and operates the Cyprus Certification Authority (CyCA).
  - –Promotes the uptake of Grid technologies in Cyprus and the deployment of new applications on CyGrid testbeds.
- **Funding agencies and projects:**
  - –EU-IST (CrossGrid, EGEE, EGEE-II, CoreGRID)
  - –EUMEDIS (Emispher)
  - –Research Promotion Foundation of Cyprus (eScience-CY)
  - –University of Cyprus

More information:

–http://cygrid.org.cy

–http://grid.ucy.ac.cy

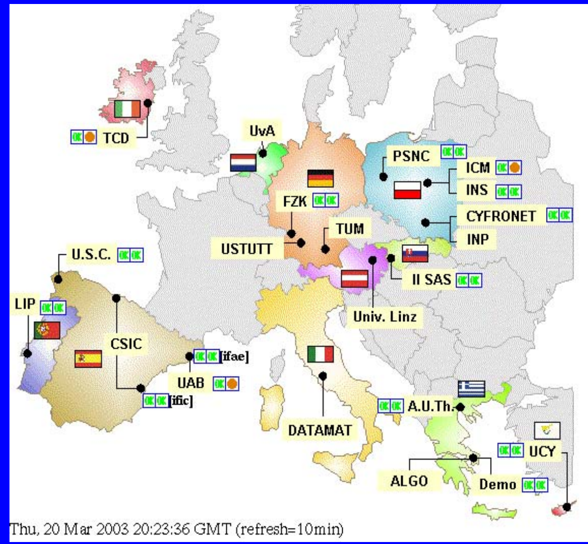
Thanks M. Dikaiakos,
Department of Computer Science

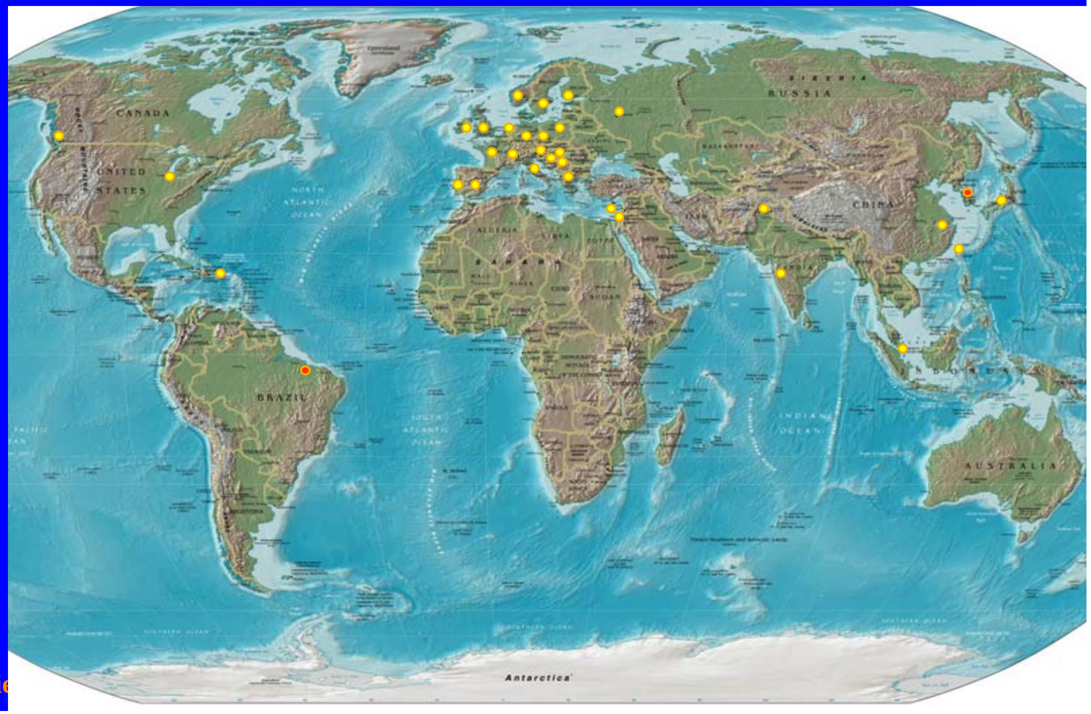
CyGrid Infrastructure

- 1 cluster: 32 CPUs, GB Ethernet, 1TB storage.
- New cluster purchased (deployment planned for January 2006):
  - 42 CPUs (IBM e326, AMD Opteron 2.2 GHz, 2GB RAM).
  - 1 GBps Ethernet
  - IBM DS400 Storage Server, FiberChannel
  - 1.5 PB Disk space
- Interconnectivity:
  - Through CyNet to Geant (155 MBps to Athens)
  - To EMISPHER Satellite Network

CyGrid in International Testbeds

- CrossGrid
- EGEE & EGEE-II
- PlanetLab (to join in 1.2005)
- Hosts the Resource Broker and Information Index of the South-East Europe Virolab of EGEE.



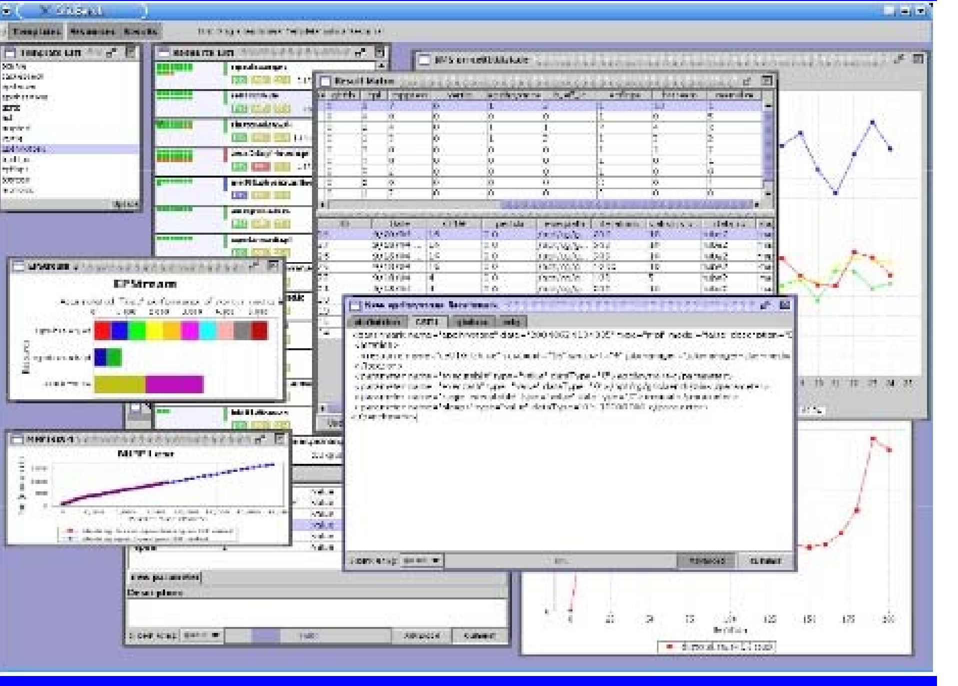


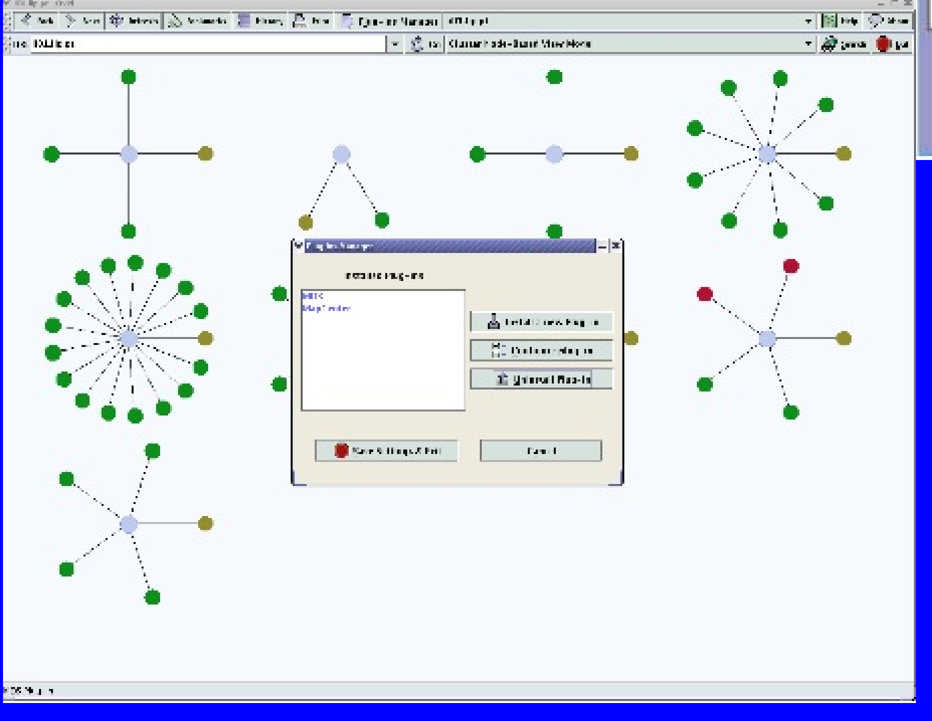
CyGrid collaboration in Cyprus

- Nicosia General Hospital (Intensive Care Unit) and Intensive Care Forum: Data-Grid applications.
- Intercollege, Cyprus: will join CyGrid and EGEE-II with a small cluster of 24 CPUs.
- Institute of Neurology and Genetics: interest in accessing EGEE testbed for thalassaemia VO.
- University of Cyprus Departments and Labs interested in applications in:
  - –Computer Science
  - –Computational Chemistry
  - –Physics

CyGrid Software

- •LCG2 & gLite middleware.
- •GridBench: a tool for auditing Grid infrastructures.
- •Ovid: a browser for navigating the Grid information space.





CyGrid Activities

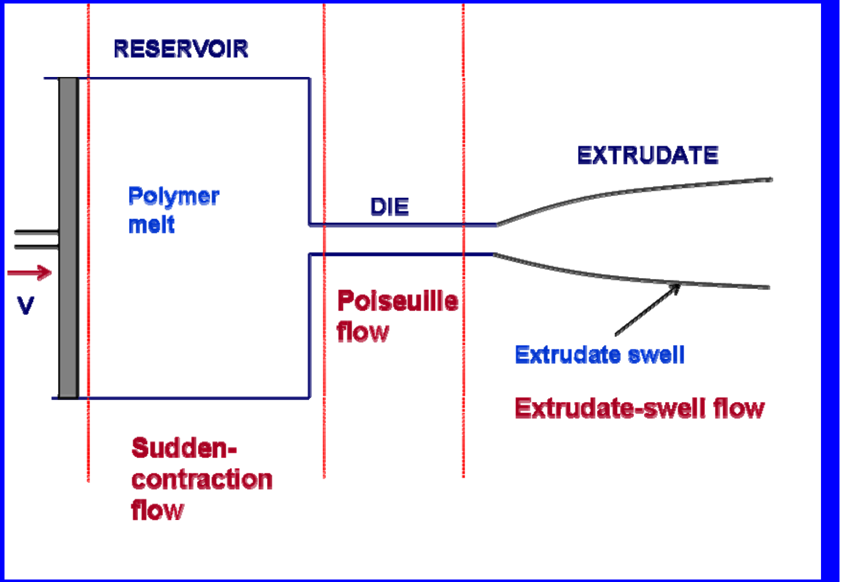
- 2nd European Across Grids Conference (AxGrids 2004), January 28-30, 2004.
- ANWIRE Winter School on Middleware. January 20-23, 2004.
- CrossGrid Workshop and Intergration Meeting. January 24-26, 2004.
- Grid Day, University of Cyprus. March 26, 2003.

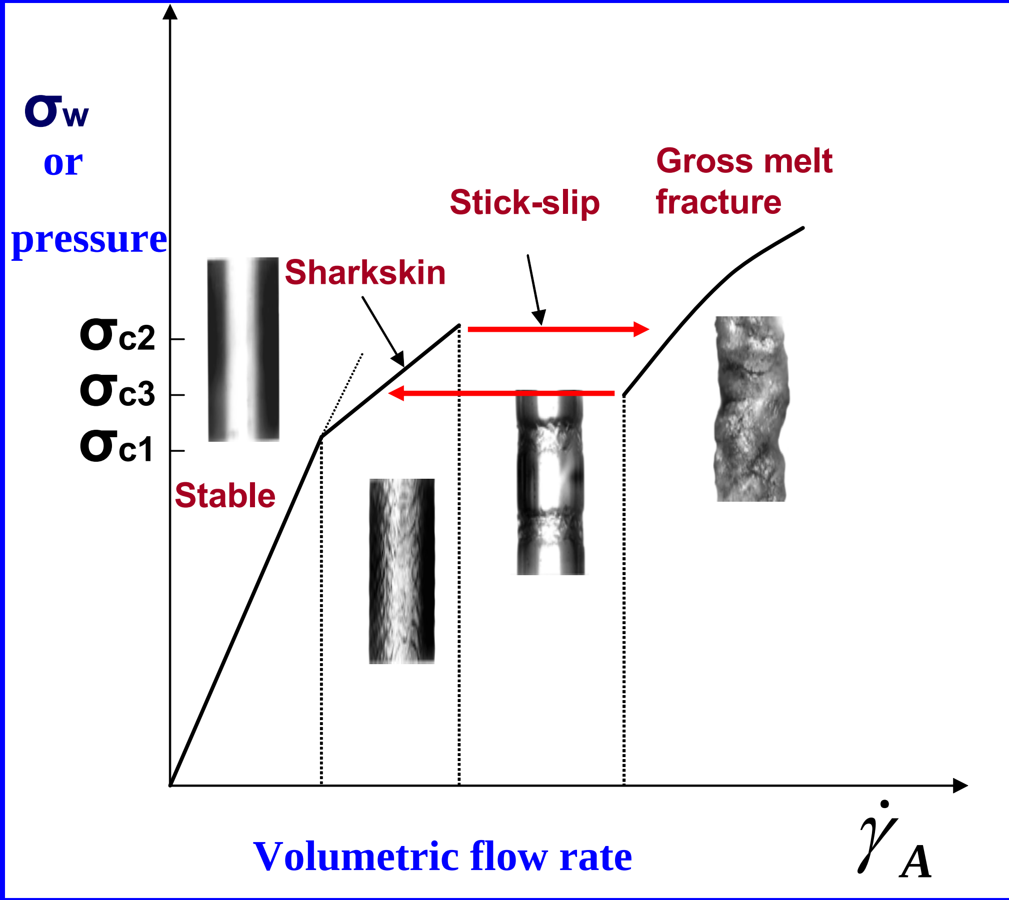
- "Information Services for Large-scale Grids: A Case for a Grid Search Engine." M. D. Dikaiakos, R. Sakellariou, and Y. Ioannidis. *Engineering the Grid: status and perspectives*, American Scientific Publishers, 2006.
- "Grid Resource Selection by Application Benchmarking: a Computational Haemodynamics Case Study." A. Tiramo-Ramos, G. Tsouloupas, M. D. Dikaiakos, P. Sloot.*Computational Science - ICCS 2005, 5th International Conference, Atlanta, GA, USA, May 22-25, 2005, Proceedings, Part I*. Lecture Notes in Computer Science, vol. 3514, pages 534-543, Springer, 2005.
- "Experience with the International Testbed in the CrossGrid Project", M. D. Dikaiakos, *Advances in Grid Computing - EGC 2005. European Grid Conference, Amsterdam, The Netherlands, February 14-16, 2005,* Lecture Notes in Computer Science, vol. 3470, pages 98-110, Springer, June 2005.

Department of Mathematics and Statistics

Computational Rheology

Two dimensional simulations of pressure and free surface oscillations in the stick-slip instability regime





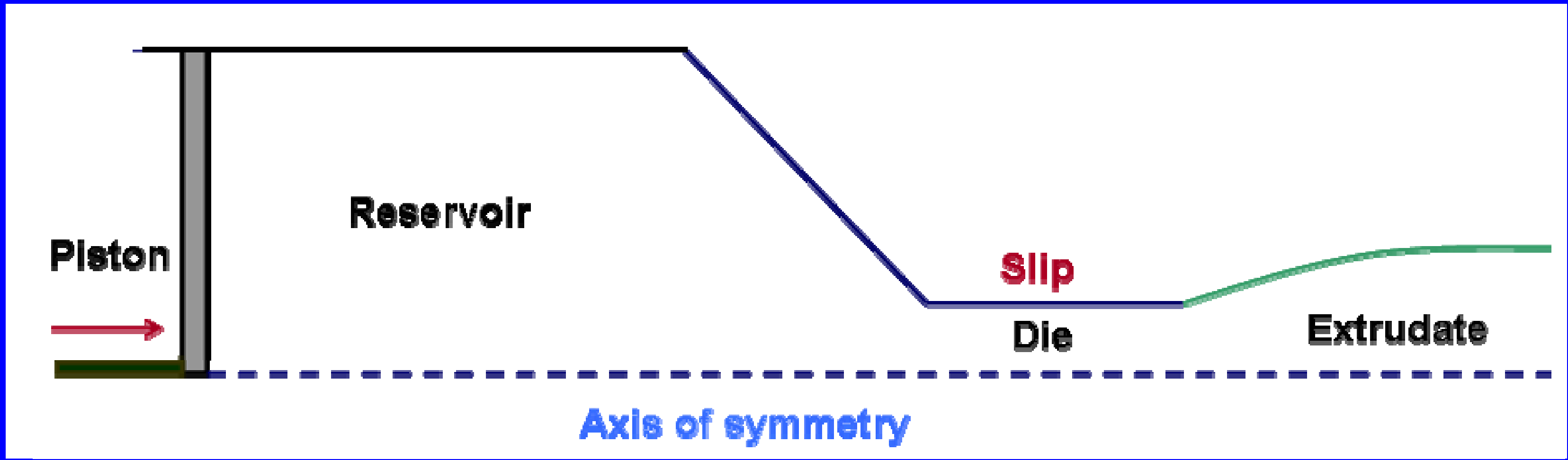
Stick-slip regime:

- **periodic pressure and mass flow rate oscillations**
- **sudden jumps of the flow rate**
- **alternating relatively smooth and distorted extrudate regions**

Thanks G. Georgiou
Department of Mathematics and Statistics
georgiou@ucy.ac.cy

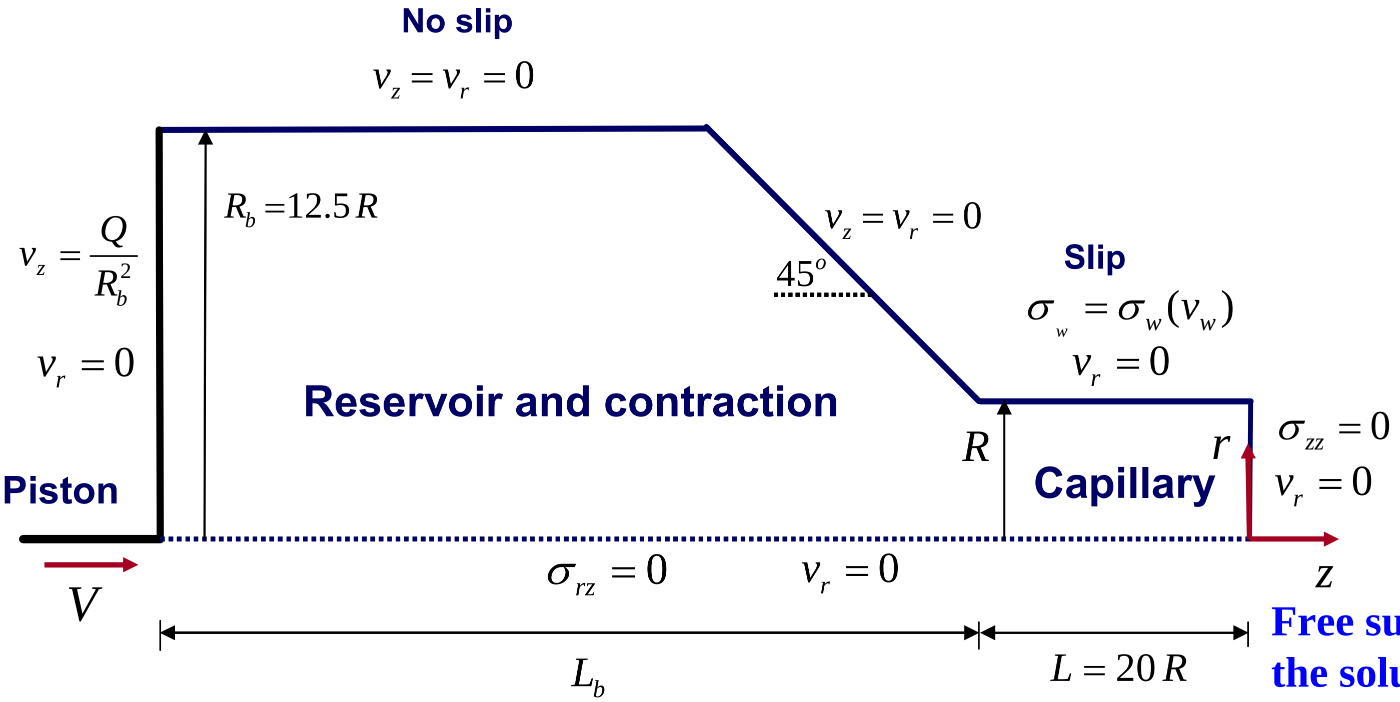
Objective

- Simulate numerically the (two-dimensional) experiments of Hatzikiriakos and Dealy (J. Rheol. 36 1992) taking into account the melt compressibility and assuming that slip occurs along the capillary wall
- Investigate the effects of the reservoir volume and the imposed flow rate on the pressure and flow rate oscillations.



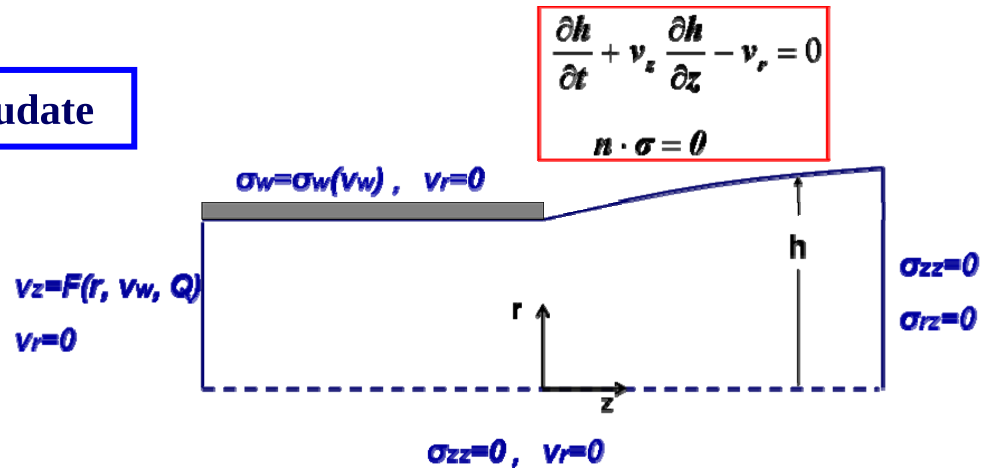
Geometry and boundary conditions

Reservoir and capillary



Free surface complicates the solution

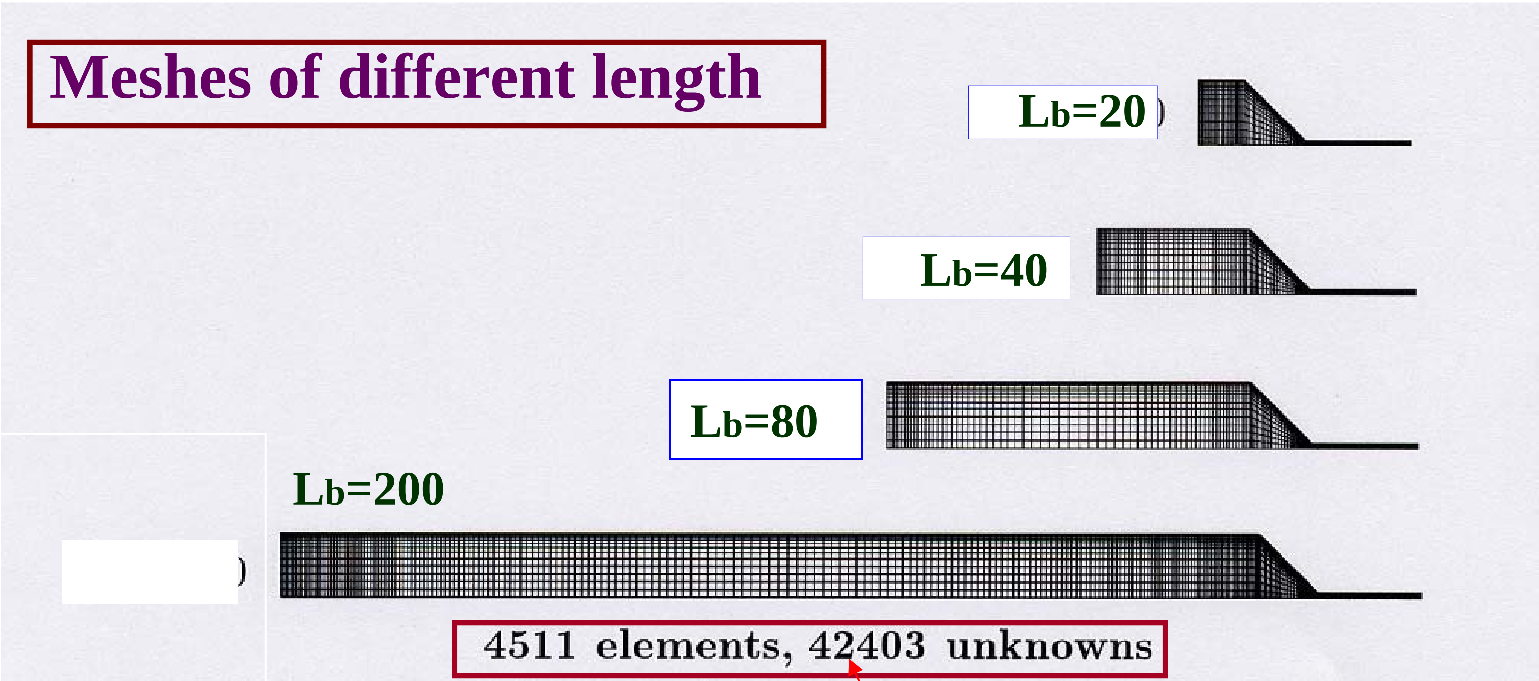
Capillary and extrudate



Must solve a coupled set of non linear partial differential equations

Numerical Method

- **Finite elements in space** (biquadratic-velocity and bilinear-pressure elements).
- **Finite differences in time** (Euler method) ~10^6 time steps
- **Full Newton iteration** (the unknown position of the free surface is calculated simultaneously with the velocity and pressure fields)
- **Frontal method** (for the solution of the resulting linear systems)



If one allows for free surface the number of degrees of freedom triples

Demonstration

Sticky-slip regime

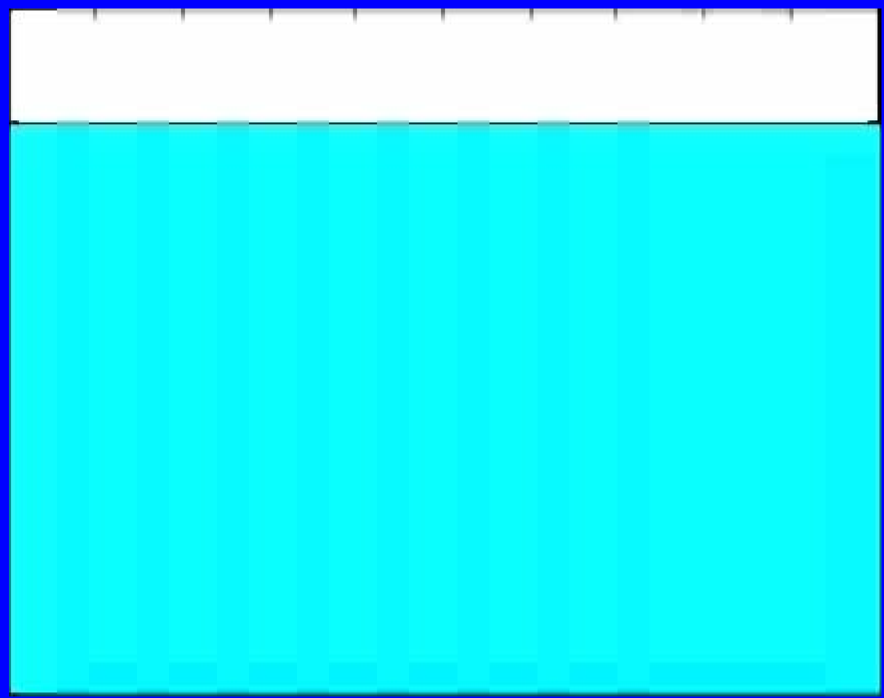
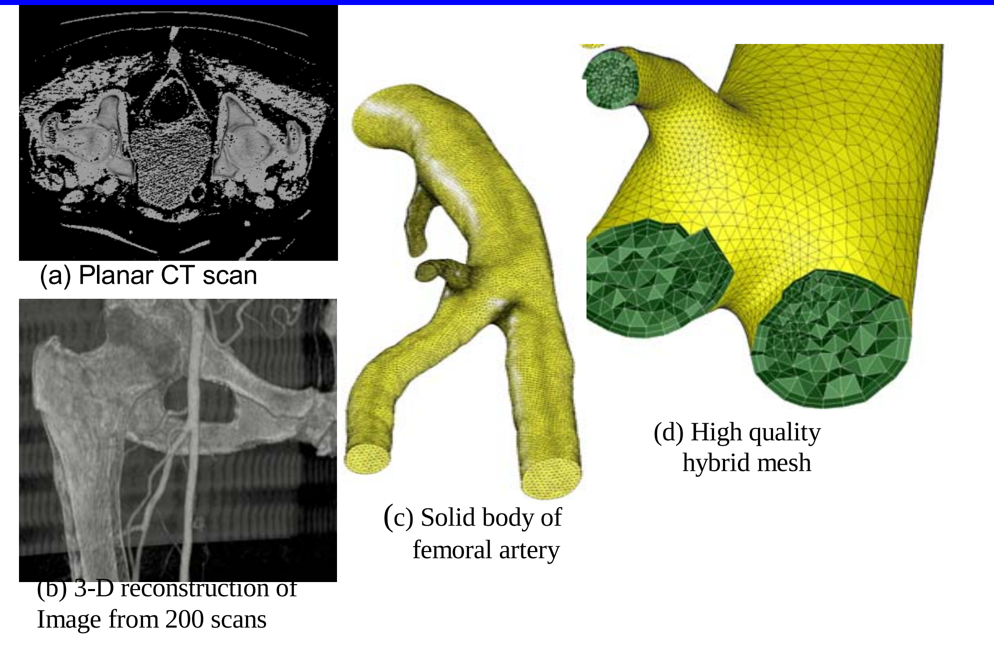
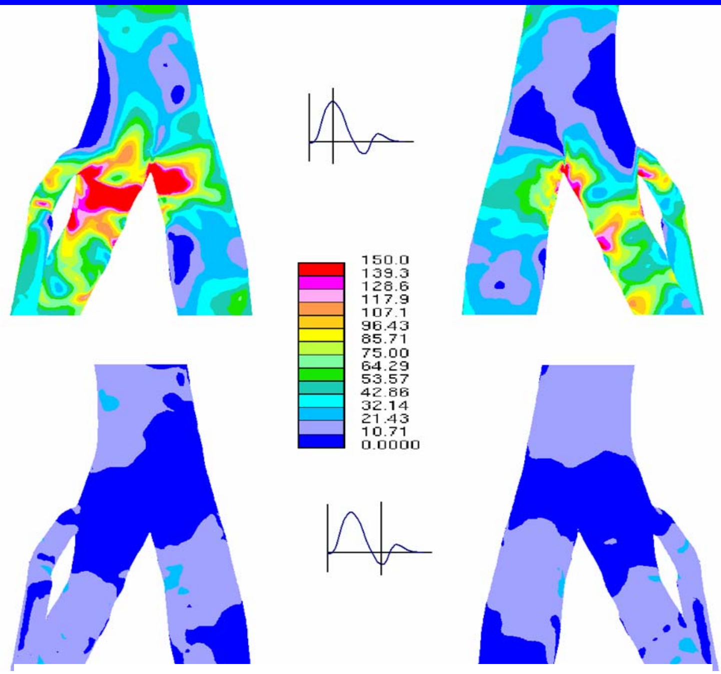


Image Based Modeling of Cardiovascular Flows

One of the goals is to perform 3-D CFD hemodynamic simulations and model the physical parameters of the flow field structure in healthy and diseased arteries



High quality mesh generation on an image-based femoral artery geometry



Wall sear stress distribution on femoral artery bifurcation model

Department of Chemistry

Computational Chemistry

- **Aims:**
  - ➢ **Compute structure, properties, dynamics of chemical systems**
  - ➢ **Augment, interpret or predict results of experiments**
  - ➢ **Design new molecules/materials**

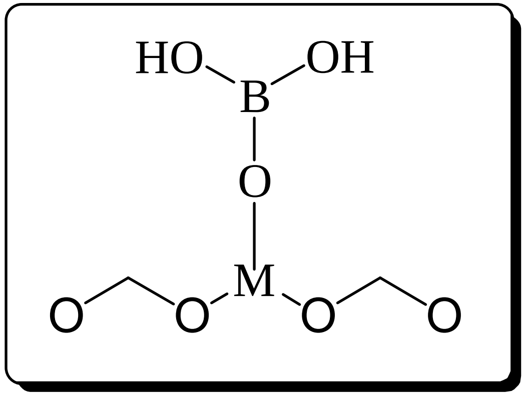
- **Methodology:**
  - ➢ **Electronic structure methods (quantum chemistry): calculate properties of individual molecules or a group of molecules**
  - ➢ **Reaction dynamics: calculate kinetic information and reaction pathways for chemical reactions**
  - ➢ **Molecular dynamics: calculate properties and dynamics of large molecules or large assemblies of molecules**

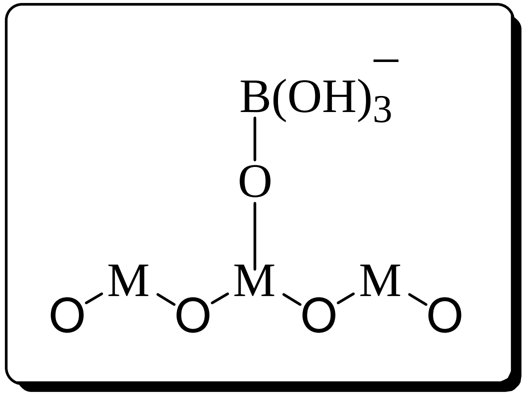
- **Computational needs:**
  - ➢ **DFT, HF methods: Fast CPUs**
  - ➢ **Coupled-Cluster methods: Fast I/O, Large (temporary) storage capacity**

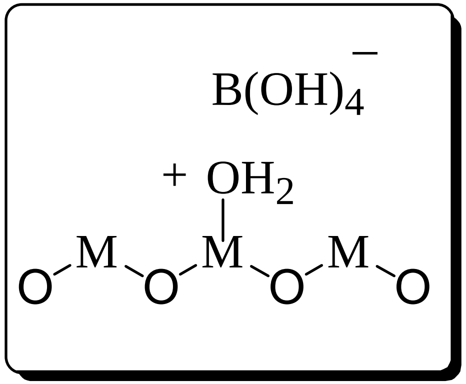
Thanks A. Nicolaides
Department of Chemistry
athan@ucy.ac.cy

Boric Acid Adsorption on Metal Oxides

M=Mg, Al







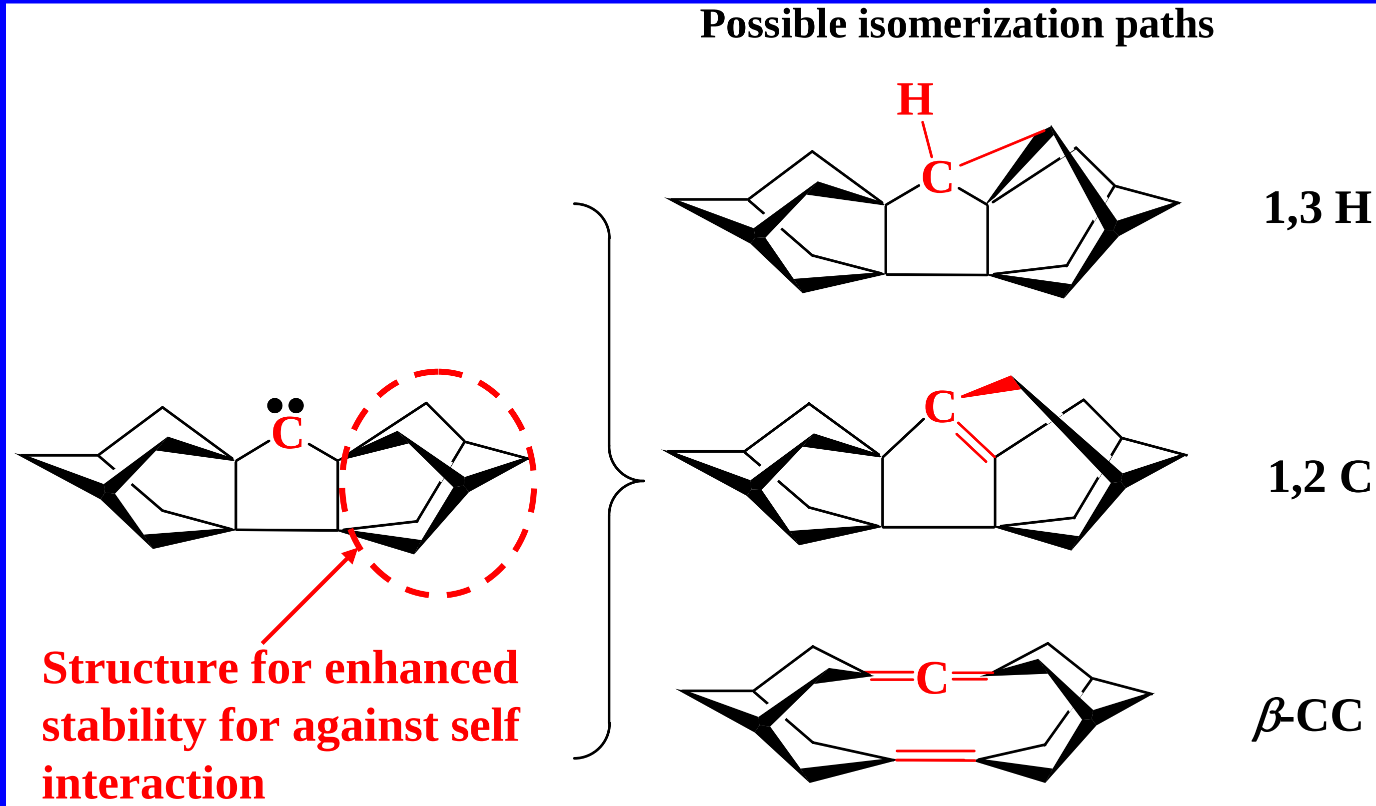
"inner-sphere"
Chemical bonding of boric acid

"outer-sphere"
Electrostatic binding of Boric acid

- **Different modes of adsorption of neutral and ionic boric acid on clays like Mg and Al oxides**
- **Estimate energetics of binding**
- **Compute IR absorptions of adsorbed species**

Application in irrigation to filter the right amount of boric acid in water

Designing Stable Singlet Carbenes



- Compute barriers of isomerization of carbenes
- Design carbenes with large computed barriers of isomerization
- Compute kinetics of isomerization

Electrolytes in Physicochemical and Biological Systems

Aim: to understand the role of electrolytes through computer simulations of model systems.

- **Numerous classical computer simulations of ions have been performed in the last 30 years.**
- **Only recently however it has been realized that proper understanding of ionic behavior close to interfaces can only be achieved by including polarizability in the classical forcefields used in MD simulations**
- **Polarizability computations are much more expensive that fixed-charge computations, and require significant computational resources.**

Systems under study:

- **Electrolyte-air interface → has been discussed in connection to biophysical applications**
- **Langmuir monolayers of lipids**
- **Salting-out of organic molecules dissolved in water**

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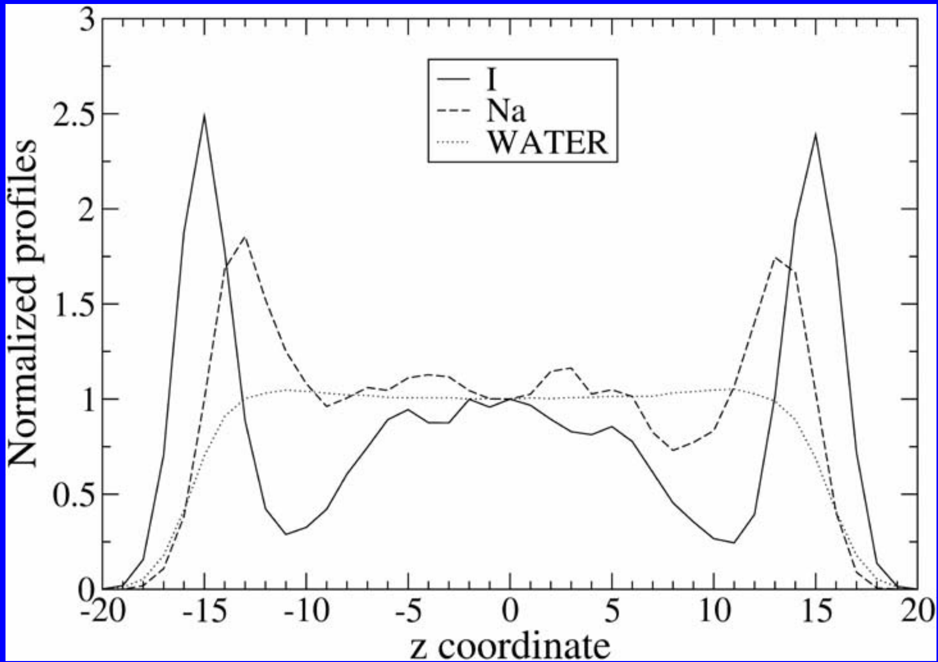
Electrolyte – air interface

- A most important model system, since no interactions exist with the second (gas) phase, and the interface acts only as a discontinuity for all interactions, creating a significant asymmetry



- MD simulations with a new polarizable model for water/ions prove that large chaotropic ions prefer interfacial solvation sites Archontis et al., JPC-B (2005)

- Cavity formation interactions favor the interfacial position. Interactions between permanent charges (Onsager model) favor the bulk. Interactions related to induced charges stabilize the interfacial location

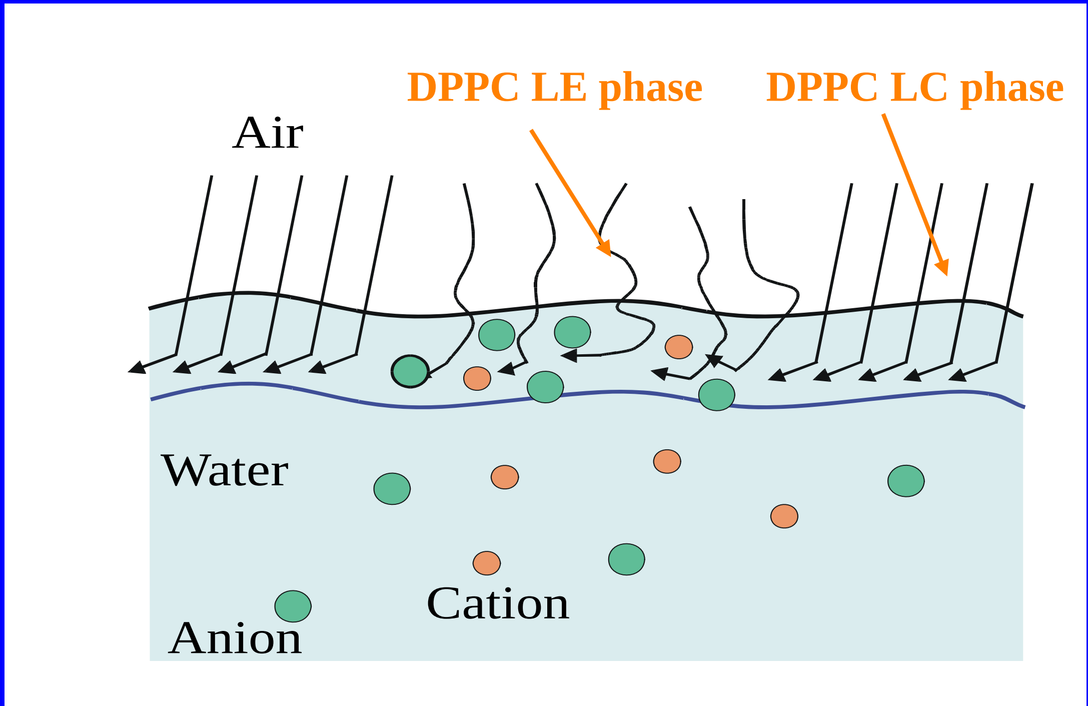
The MD simulations were run in small systems (1000 water molecules with 22 ions of each sort, typical of NaCl concentrations in seawater), and for rather short times (2-4 ns):

- Equilibration is not perfect (asymmetry in graph, pair correlation function should go to unity in the middle of the water slab)

- To check the validity of the results one needs to run the simulations in larger systems (one order of magnitude) and for much longer times

Access to supercomputers necessary

Langmuir monolayers of lipids



► These systems are important biological membrane-mimetic models and go one step beyond the free air-water surface. Interfacial binding interactions are now possible. Possible also to easily tune interfacial density of interaction sites.

► For the important cell-membrane lipid DPPC experiment shows that: The disordered liquid-expanded (LE) phase is affected by ions, but the ordered liquid-condensed (LC) phase is not affected.

Theoretical calculations revealed that ions partition into the lipid LE phase, and the partition coefficients can be evaluated from the experimental data combined with appropriate models.

Two issues remain unresolved and must be probed with large scale MD simulations:

► How do the large polarizable ions interact with the lipid monolayer? Such a calculation has never been performed with polarizable forcefields.

► Do some ions affect the average headgroup tilt of the phospholipids at the air-water interface? By what mechanisms and to what extent?

These questions require large system simulations and supercomputers

Salting-out of organic molecules dissolved in water

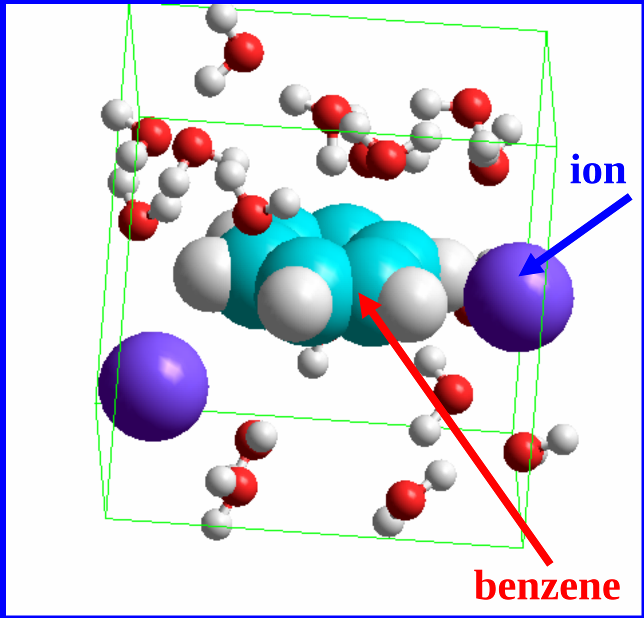
- **Very important problem for chemistry, environmental science and biology**

The problem is related to the precipitation of organics in environmental waters, to the purification of organic chemicals and proteins, and to the precipitation of kidney stones.

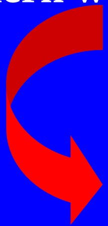
Investigations of the salting-out effect will prove if the same surface chemistry ideas, that were applied to the free water surface or to monolayers of lipids, can also be applied to solution physical chemistry.

Is polarizability again the really important factor?

Can we treat small organics as impurities/surfaces within an electrolyte solution?



- **Small-scale computations with one solute in an electrolyte solution can be run on modern workstations**



Larger systems and/or longer simulation times require supercomputer resources.

Conclusions

•The Physics, Computer Science and Engineering Departments have small scale computer facilities

•However larger applications require access to supercomputers faster of many orders of magnitude outside Cyprus

•Many other applications from Chemistry, Mathematics, Bioinformatics are in need of supercomputers

➡ **A European facility will be welcome by researchers in Cyprus**

Many thanks to Th. Lippert and N. Attig for this initiative and invitation for us to take part