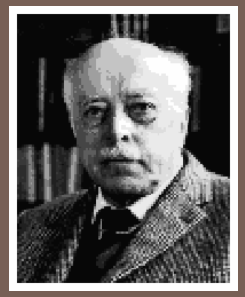
National Institute for Research and Development of Isotopic and Molecular Technologies

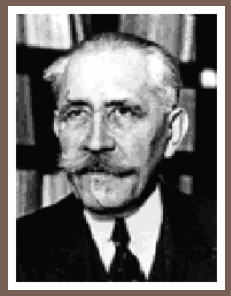
# High-Performance and Grid Computing at INCDTIM, Cluj-Napoca, Romania

Călin G. FLOARE | Felix FĂRCAȘ | Gheorghe ADAM



Max von Laue

1879-1960



Paul Langevin

1879-1946

Joseph Fourier

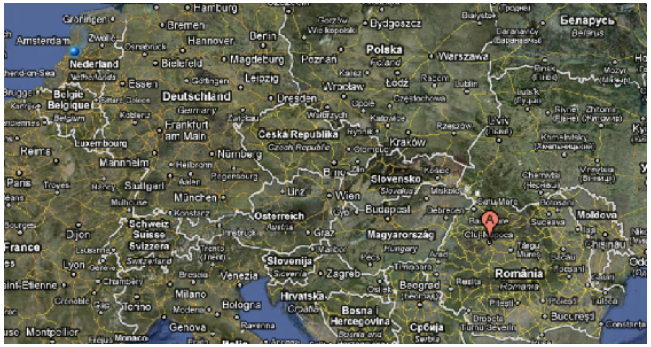
1768-1830

The 6th International Conference "Distributed Computing and Grid-technologies in Science and Education, 2014, Dubna, Russia

# Outline

- Introduction
- GRID site & IBM iDataPlex cluster
- Applications in our Laboratory
  - The story of a serendipitous discovery
- A short view on the future of efficient and reconfigurable computing
  - ARM-based cores & x86 CPUs embedded with reconfigurable chips

# Cluj-Napoca - Romania


Cluj in 1617 - Bird's eye view by Georg Houfnagel after a painting by Egidius van der Rye.

The city center - air view from south-west (1930)

# NIRDIMT, Cluj-Napoca

## Research Departments

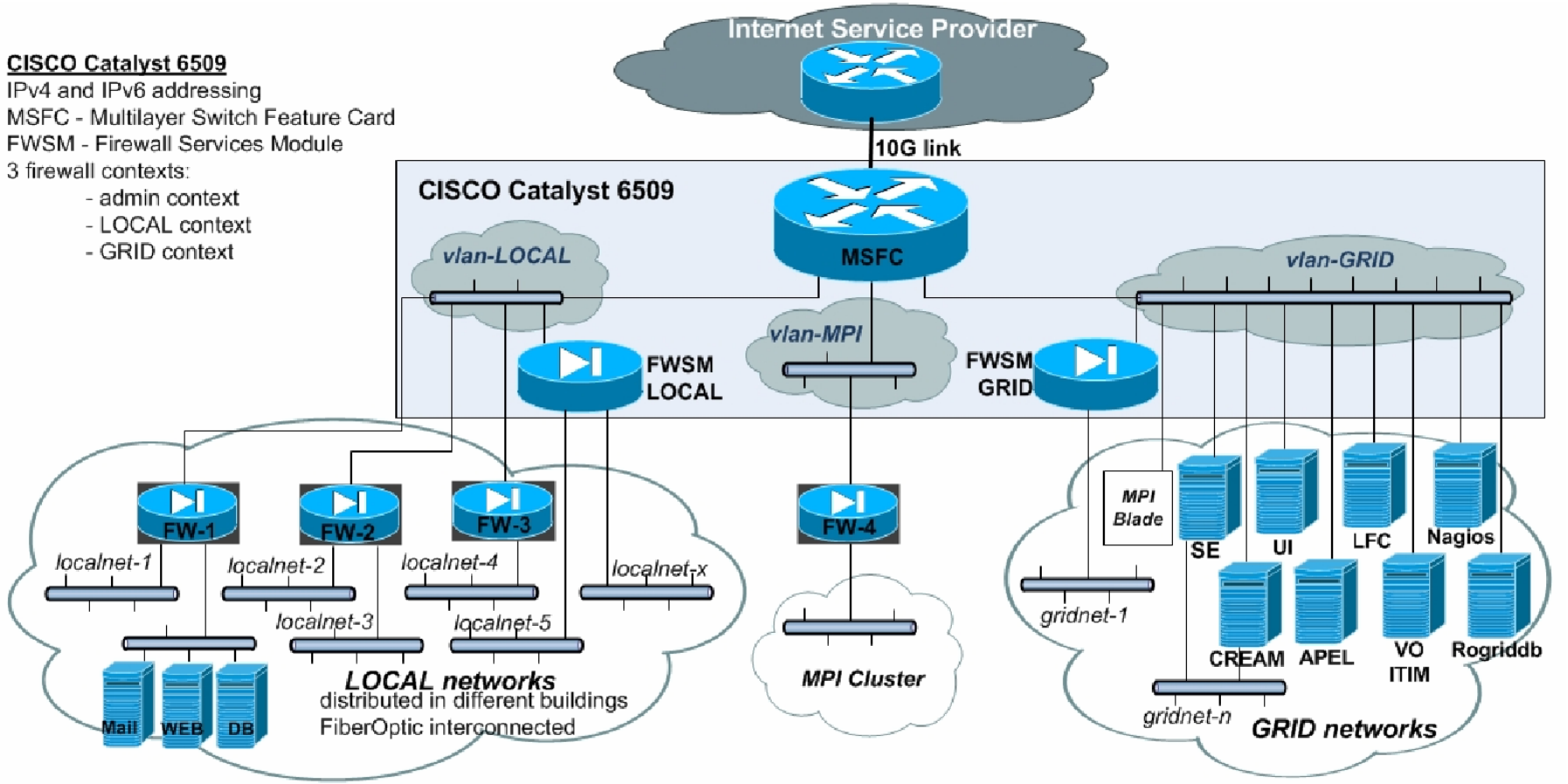
- Isotopes separation and labeled compounds
- Mass spectrometry, chromatography and ion physics
  - High-Tech Engineering in ATLAS experiment at LHC Cern Geneva (team4)
- Molecular and Biomolecular physics
  - Numerical Modeling
  - Structural Analysis in Solids
  - Self-Assembled Molecular and Biomolecular Systems
- Physics of multifunctional nano-structured systems

## Data Center

- RO-14-ITIM Grid site
- IBM iDataPlex HPC cluster


http://itim-cj.ro/brosura2013/en/

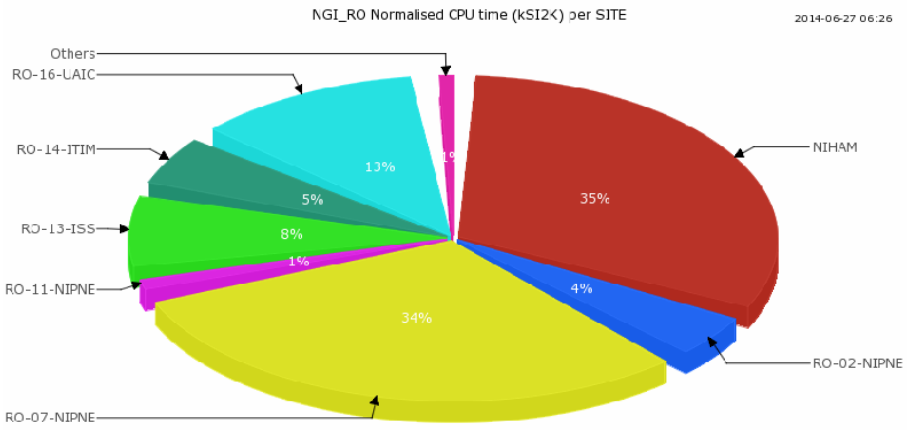
# Datacenter Logical Map

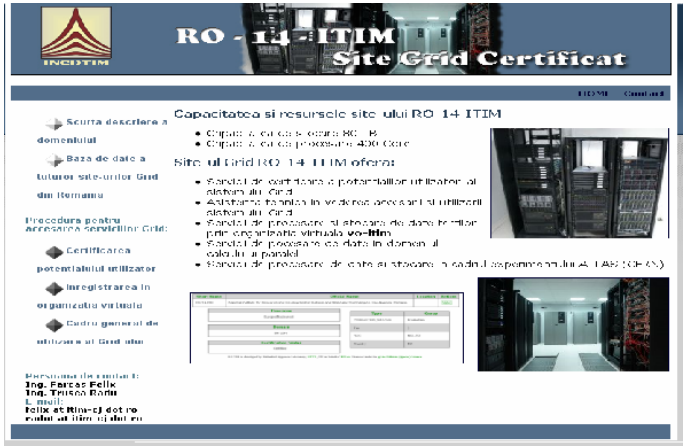


# RO-LCG and RO-14-ITIM

## RO-LCG

- is a consortium of five institutions which represents the Romanian contribution to the WLCG collaboration.
- was created in March 2006, when the WLCG Memorandum of Understanding was signed.
- is funded through R&D projects by the Romanian National Authority for Scientific Research.
- hosts and operates most of the national Grid resources, providing 98% of the Romanian Grid production.




http://grid.itim-cj.ro

- LHC VO distribution of Normalised CPU time (kSI2K) grouped by SITE and VO

| Normalised CPU time [units 1K.SI2K.Hours] by SITE and VO | | | | | |
|---|---|---|---|---|---|
| SITE | alice | atlas | lhcb | Total | % |
| NIHAM | 32,061,631 | 0 | 0 | 32,061,631 | 34.57% |
| RO-02-NIPNE | 0 | 4,168,107 | 0 | 4,168,107 | 4.49% |
| RO-07-NIPNE | 6,164,151 | 18,139,730 | 6,769,535 | 31,073,416 | 33.51% |
| RO-11-NIPNE | 0 | 0 | 945,506 | 945,506 | 1.02% |
| RO-13-ISS | 7,212,749 | 0 | 0 | 7,212,749 | 7.78% |
| RO-14-ITIM | 0 | 4,908,062 | 0 | 4,908,062 | 5.29% |
| RO-15-NIPNE | 0 | 0 | 742,445 | 742,445 | 0.80% |
| RO-16-UAIC | 24 | 11,626,514 | 0 | 11,626,538 | 12.54% |
| Total | 45,438,555 | 38,842,413 | 8,457,486 | 92,738,454 | |
| Percentage | 49.00% | 41.88% | 9.12% | | |

# GRID Site - RO-14-ITIM

- On-line CPUs: **440 cores**
  - *Hewlett Packard Blade C7000 with 16 Proliant BL280c G6*

    *2 Intel Quad-core Xeon x5570 @ 2.93 GHz, 16 Gb RAM, 500 Gb HDD*
- Storage capacity: **57 TB**
- Virtual Organization (**ATLAS, ops, voitim**)
- Operation system Scientific Linux 6.4 x86-64
- As Middleware we use EMI v3
- Network Link: RoEduNet 10 GB from 2011

# iDataPlex Cluster

## IBM dx360 M4

- 64 × Intel Xeon Eight-Core CPU E5-2665 @ 2.40GHz
- 4 × Intel Xeon Eight-Core CPU E5-2670 @ 2.60GHz
- 2 × nVIDIA Tesla M2090 GPUs
- 64 GB / node
- Mellanox Infiniband FDR (56GB/s)
- Storage 14 TB GPFS
- Red Hat Enterprise Linux Server release 6.3 (Santiago)
- Batch system: IBM Platform LSF 8.3


- *Quantum Chemistry & MD codes*
  - AMBER
  - CPMD, CP2K
  - GAMESS
  - Gaussian
  - GROMACS
  - LAMMPS
  - MOLPRO
  - NAMD
  - DFTB+
  - Siesta
  - CRYSTAL
  - Quantum Espresso
  - VASP
  - Accelrys Materials Studio

# Monitoring and Protection System

- Temperature (20 - 23 °C)
- Humidity
- Fluid detector
- Smoke detector

UPS APC Symetra 160 kVA

Power generator 275 kW

# Financial Resources

- Fund through National Authority for Science Research (ANCS)
- PN2-Capacities-M3 CERN / CONDEGRID: National contribution to the development of the LCG computing grid for elementary particle physics (12EU/2009)
- Continuing the 15 EU / 2009-2014
- Cooperation program "Hulubei-Meshcheryakov" together with the Laboratory of Information Technologies at JINR –Dubna 2010-2014
- **POS-CCE 192**, *Improving the capacity and reliability of INCDTIM GRID center for integration in international networks (INGRID)*
- POS-CCE 536, Axis 2, operation 2.1.2
- PN-II-RU-TE-2011-3-0124 : *„Dynamics of Molecular Excited States in interaction with coherent pulsed radiation"*
- PN-II-RU-TE-2011-3-0085: *„First-principles Modeling of $SrTiO_3$ Based Oxides for Thermoelectric Applications"*
- **PN-II-KAI2.2- O2.2.1-2PM/2008**: *Molecular and Biomolecular Physics Department Upgrading - MDFMOLBIO*

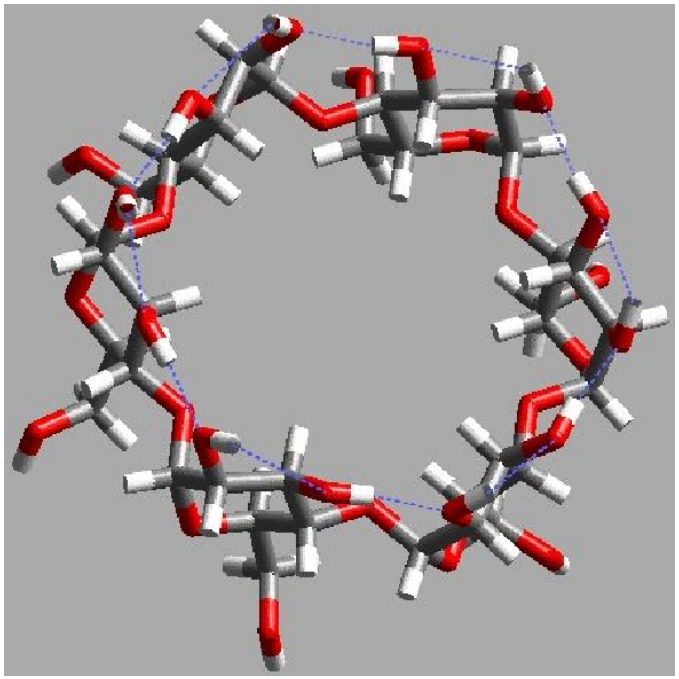
# Applications in our laboratory

- First-principles Modeling of $SrTiO_3$ Based Oxides for Thermoelectric Applications
- Density Functional Theory (DFT) Study of Trioxotriangulene derivatives in bulk state, NanoElectronics
- Time-Dependent DFT study of tautomerism and proton transfer in photoionized species
- Crystalline structural investigation of Polymorphic Compounds
- Modeling of XUV and soft X-ray production through high-harmonic generation in atomic and molecular gases
- Human Aquaporin & H-Ras Peptide Nanoclusters Molecular Dynamics Simulations
- Macromolecular and Biomolecular associations
- Satellite Imagery Processing Algorithms - see the talk of Prof. Gh. Adam on Thursday

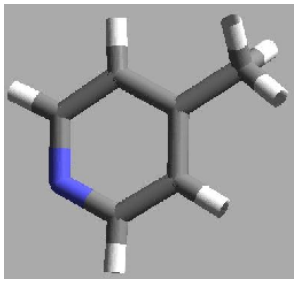
...

# The story of a serendipitous discovery[1]

$\alpha$-cyclodextrine, $\alpha$CD:
the association of 6 glucose units: $(C_6O_5H_{10})_6$

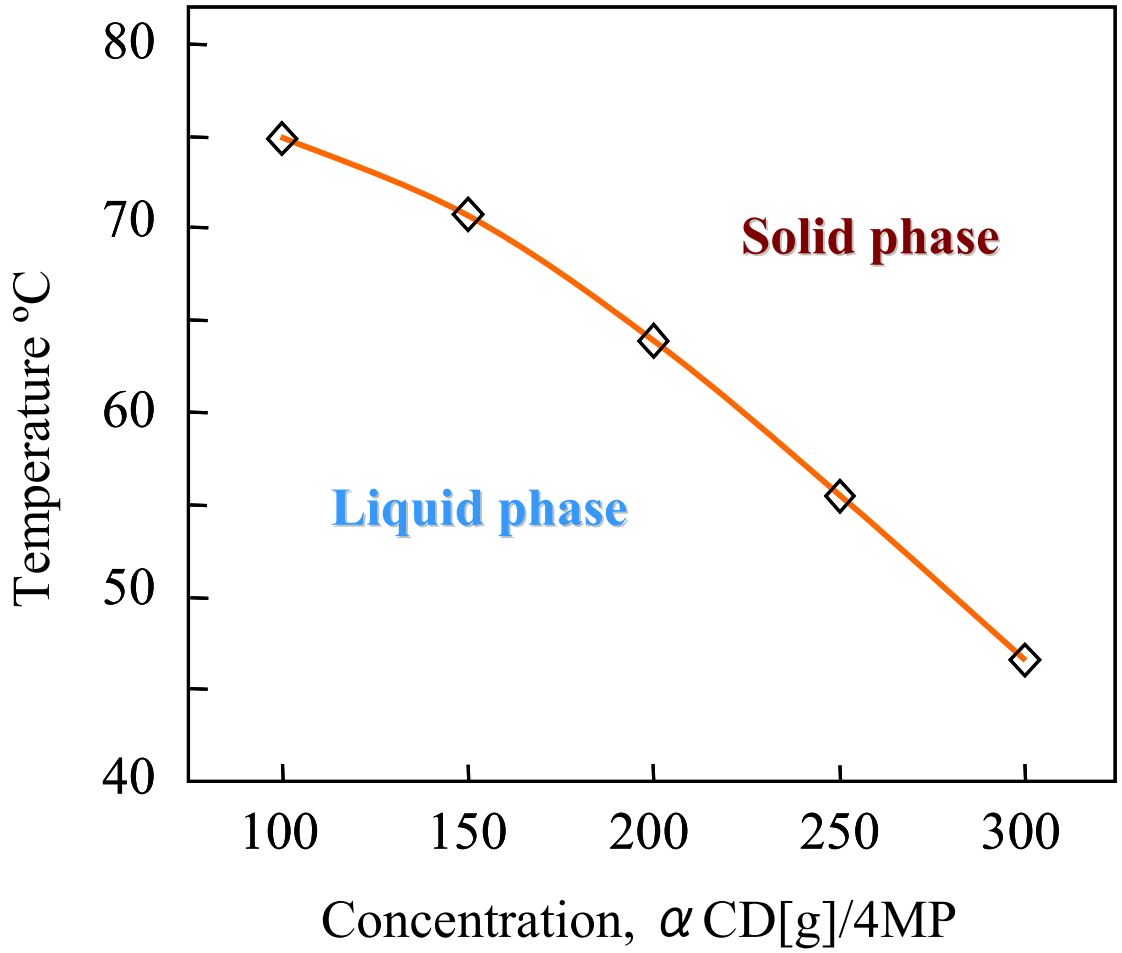


4-methylpyridine, 4MP:
$C_6NH_7$



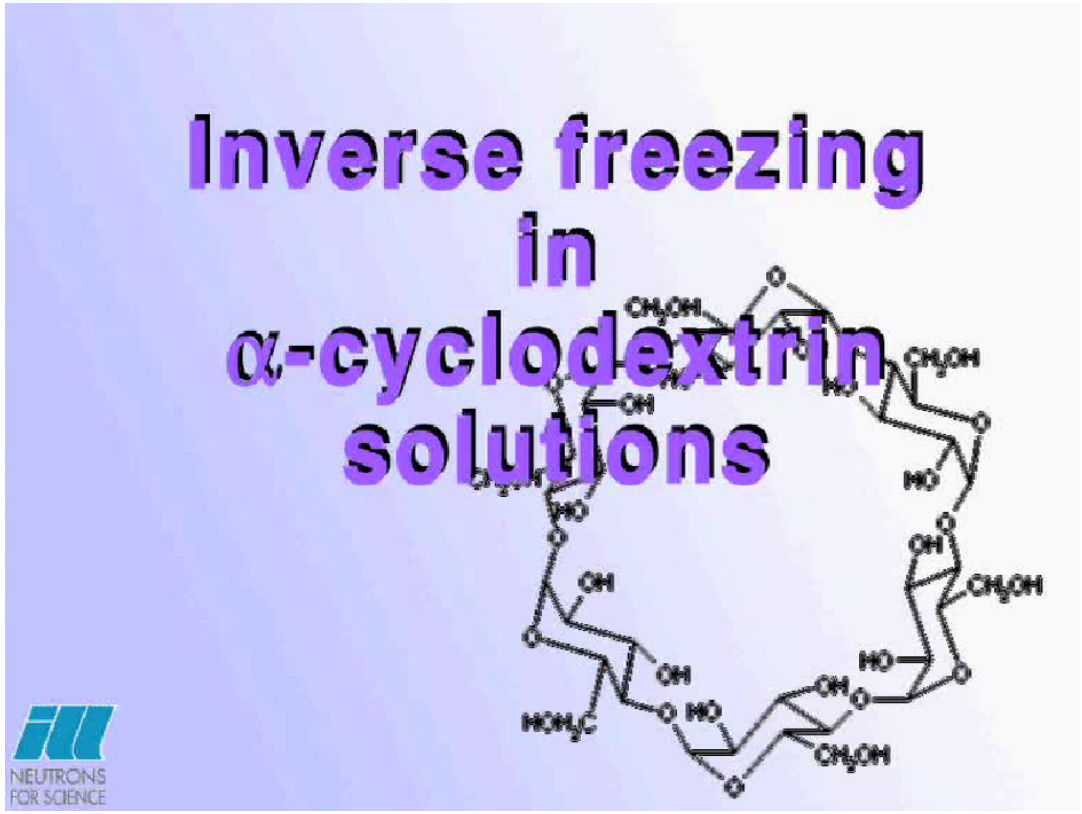
…..and a bit of water

[1] M. Plazanet, **C. Floare**, M. R. Johnson, R. Schweins, H. P. Tommsdorff, *Freezing on heating of liquid solutions*, J. Chem. Phys., 121(11), 5031 (2004), ILL Annual Report 2004, 54-55 and the papers which followed.




Stoichiometry: 200g/l ~ 1 α CD for 50 4MP

# A movie by A. Filhol, Laue-Langevin Institute

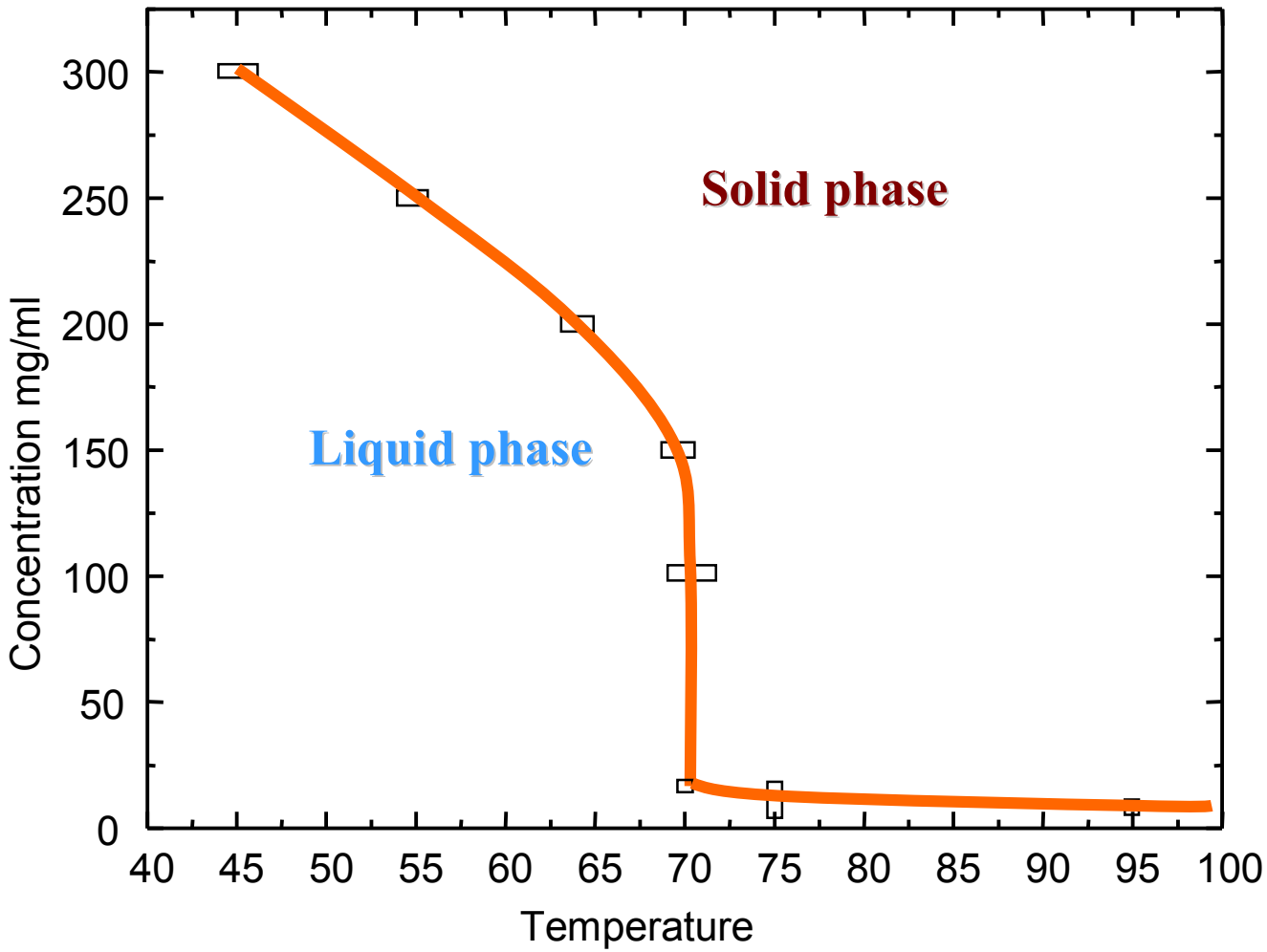



Azobenzene : melts at 66°C

αCD-4MP : freezes at 66°C

http://www.ill.eu/about/movies/experiments/in16-a-liquid-paradox

# Solubility of αCD in 4MP

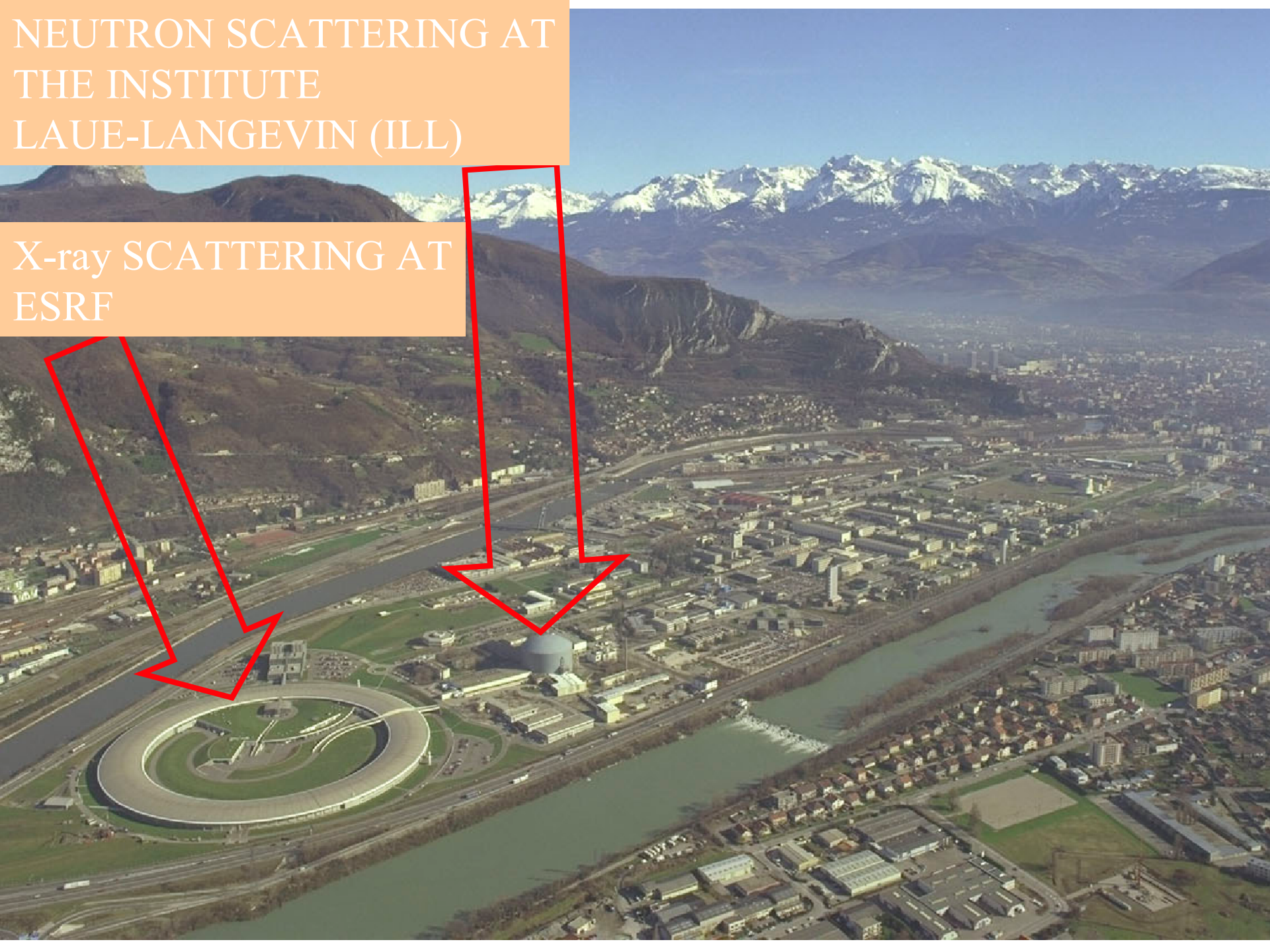


# How we can rationalize these surprising observations?

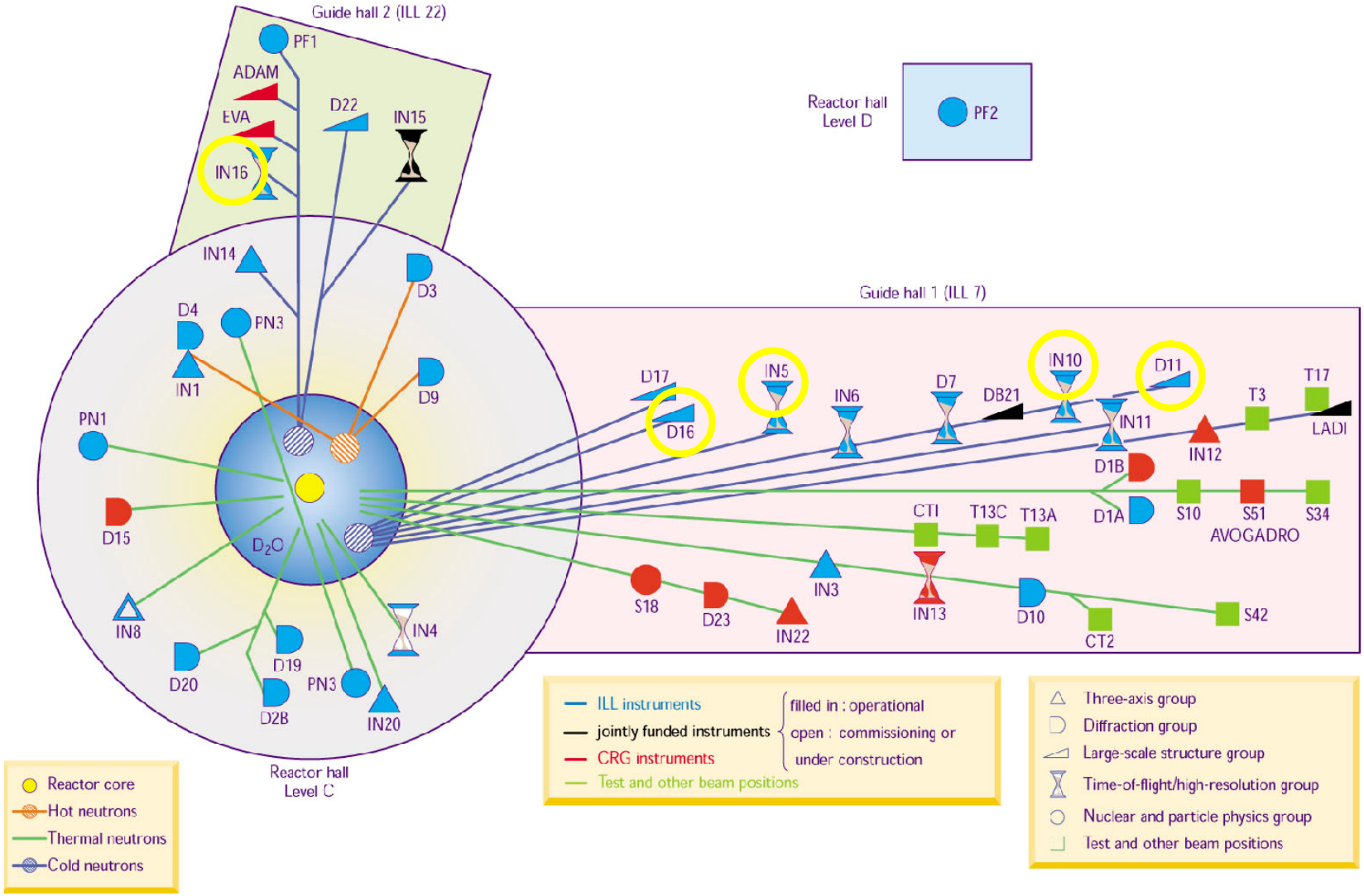
As temperature increases, entropy must increase, how is this compatible with the observation that crystalline order is established and that molecular motions are slowed down?

Characterize the changes of the structure and of the molecular dynamics by:

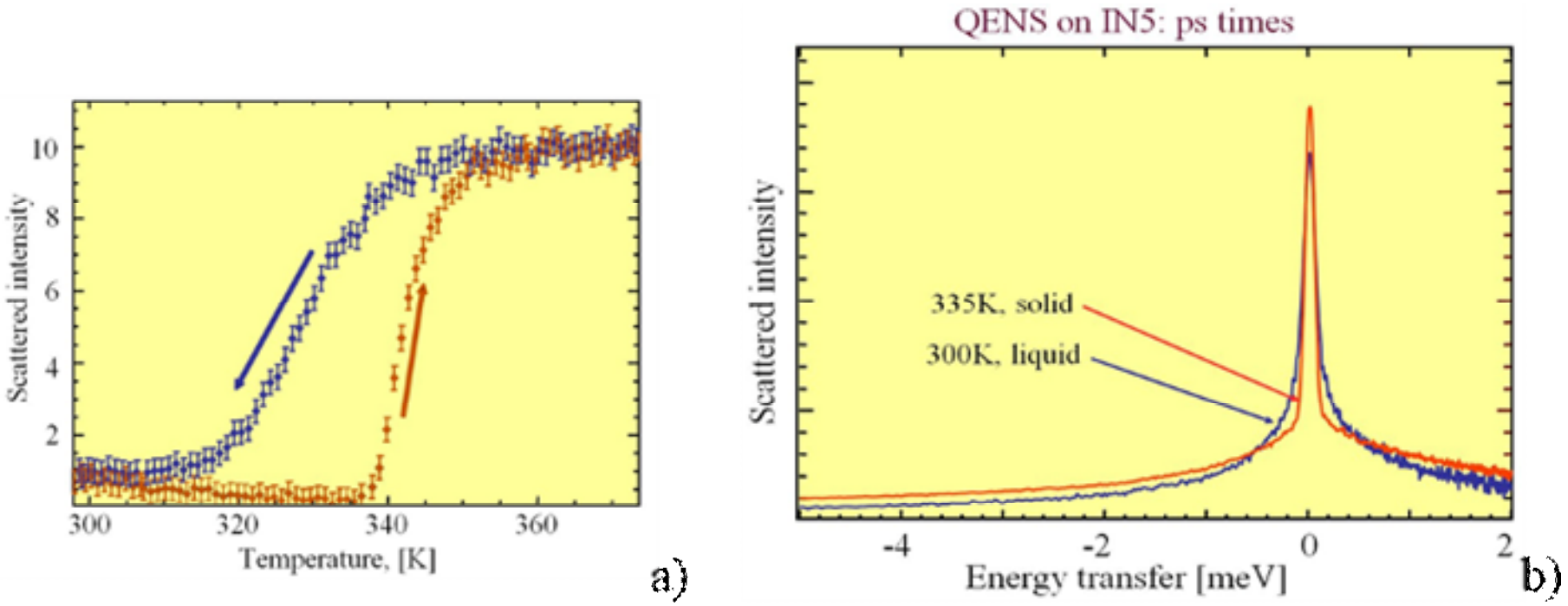
- elastic and inelastic neutron scattering
- neutron and X-ray diffraction,
- low-field NMR and
- molecular dynamics simulations


NEUTRON SCATTERING AT THE INSTITUTE LAUE-LANGEVIN (ILL)
X-ray SCATTERING AT ESRF

# Instruments Used



# Results obtained on IN10 and IN5

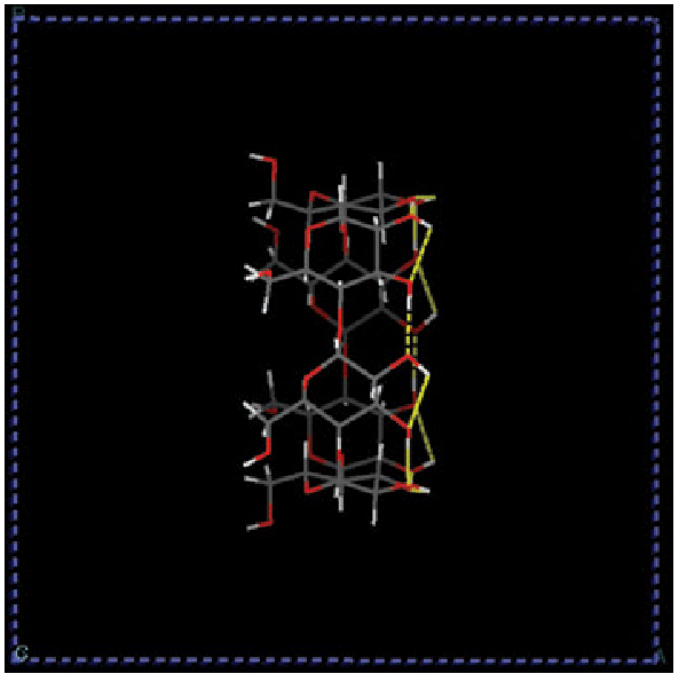



a) Hysteresis-like fixed window (elastic) scan, IN10, ILL; b) Quasi-elastic neutron spectra, IN5, ILL

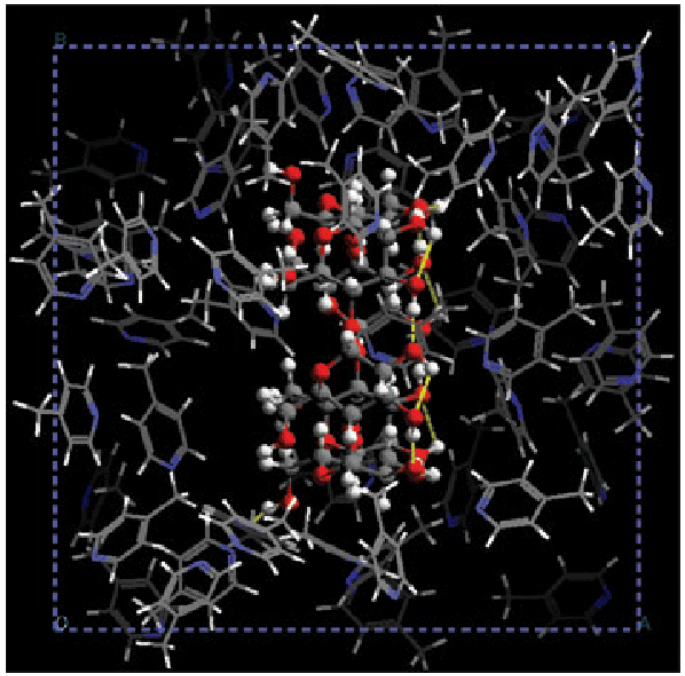
# Model system studied initially

- 2004 - NPT molecular dynamics simulations using Accelrys CERIUS$^2$ v4.6 with COMPASS forcefield running on different SGI workstation
- A periodic box with the dimensions 24Å × 24Å × 24Å, containing:
  - ❖ one α-CD molecule
  - ❖ 50 molecules of 4MP

➡ 826 atoms



(a)



(b)

# A more appropriate description

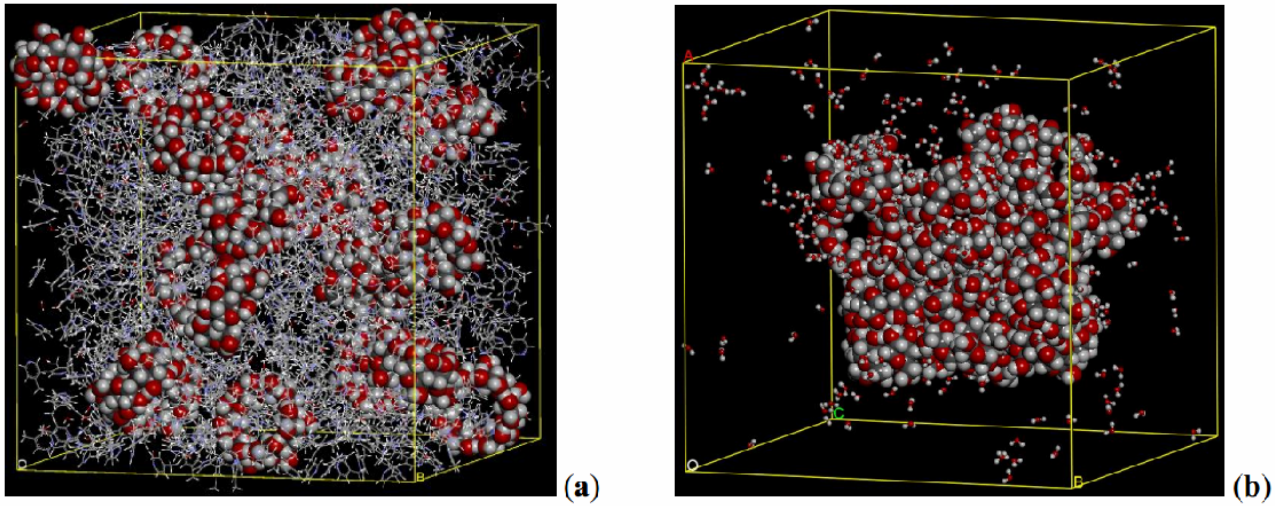
HPC-Europa2
Pan-European Research Infrastructure on High Performance Computing

**2011-2013**

- 20 aCD molecules
- 1120 molecules of 4MP
- 240 water molecules
- NPT ensemble MD using AMBER
- $(60\ Å)^3$ box
- match the experimental molecular ratio (200 mg aCD per ml 4MP)

→ **18920 atoms**

- speed of 0.22ns/day (1 core), 0.39ns/day (2 cores) and 0.69/day (4 cores)
- 22ns/day when using 256 cores, on a system containing around 23500 atoms an AMBER benchmark on IBM SP5 cluster (IBM p575 Power 5, bassi.nersc.gov, 118 8-cpu nodes, 1.9 GHz Power 5+ cpu, 2 MB L2 cache, 36 MB L3 cache, 32 GB memory per node)
- ~24ns/day running on 2×Tesla M2070 GPUs on a single node of CINECA PLX cluster




Snapshots of the simulation box at 300K (a) and at 370K (b).

# Analysis

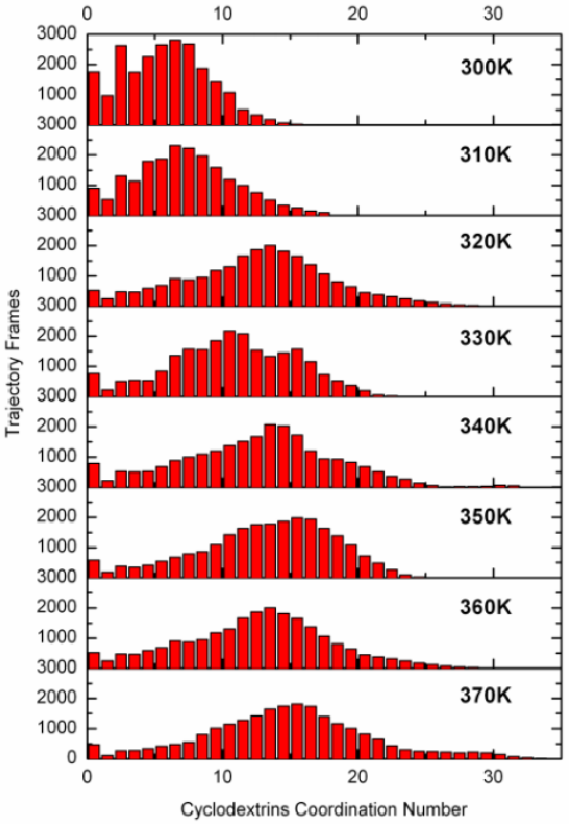
- 100 ns NPT trajectories at 8 different temperatures
- PLUMED plugin implemented in GROMACS was used to compute the cyclodextrin coordination number

We continue with:

- Hydrogen-bond dynamics and cluster formation analysis
- (Generalized) Correlation coefficients
- Optimize the force fields using *force-matching method*
- We need to simulate a bigger system

This study has been performed under the HPC-Europa2 project (project number: 228398) at SISSA and CINECA, Italy.

http://bit.ly/cfloaremdfreezing

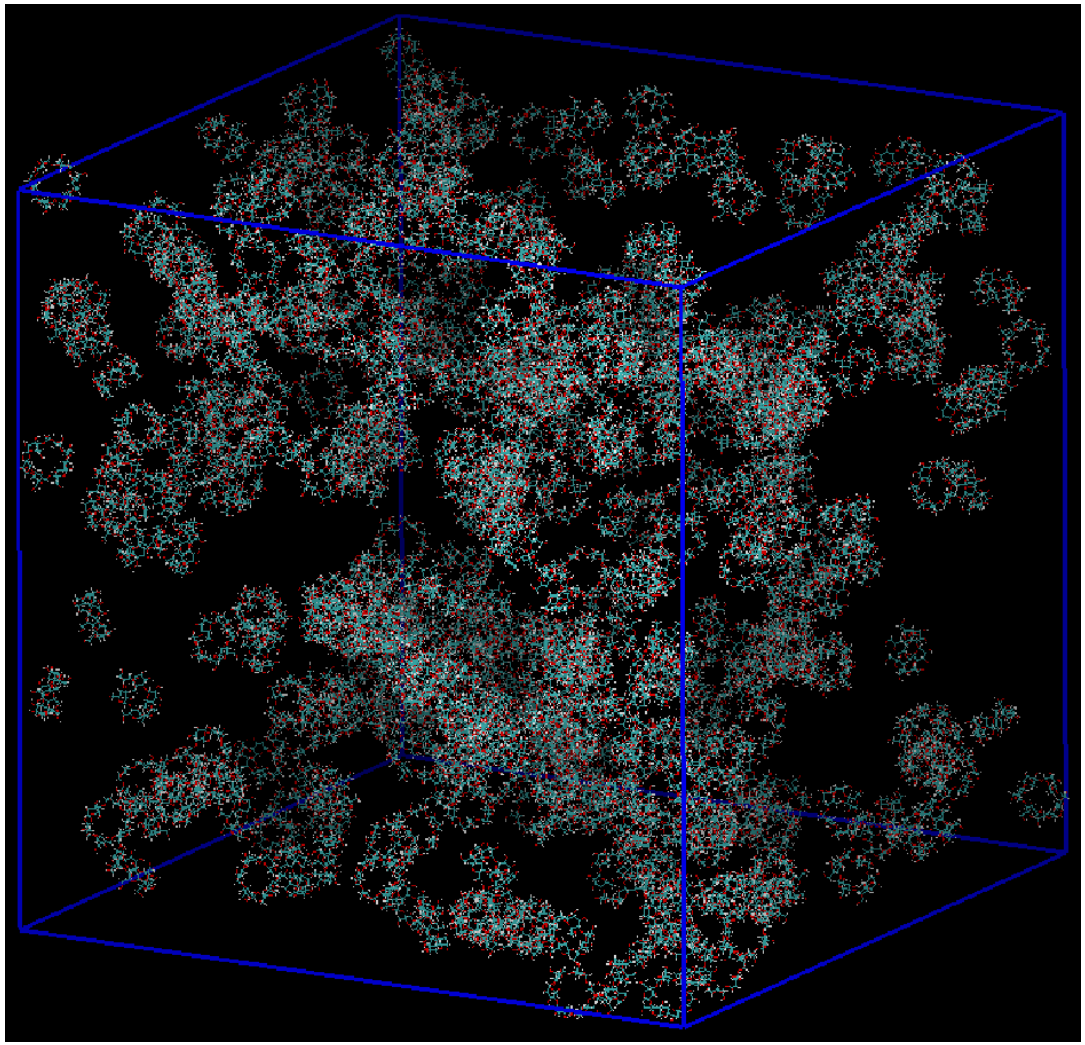



Cyclodextrin coordination number along the 100 ns trajectories at all simulated temperatures

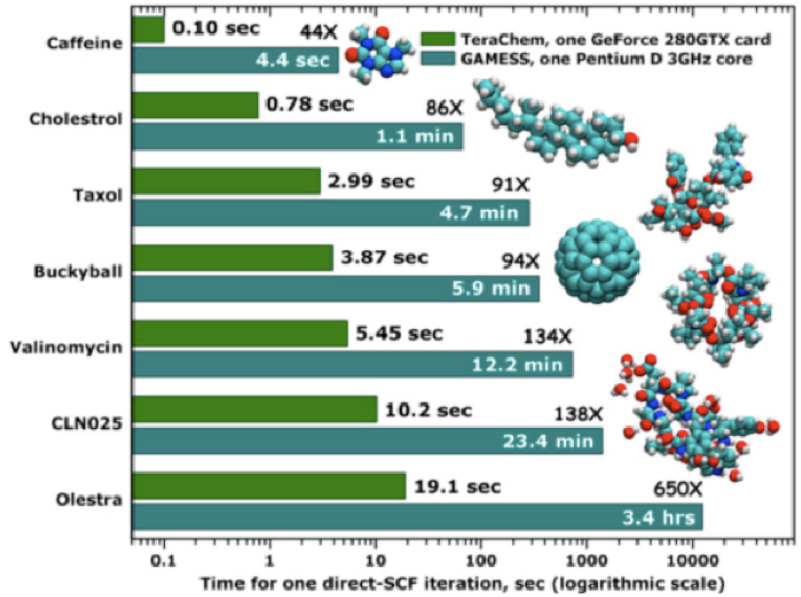
# Actual system

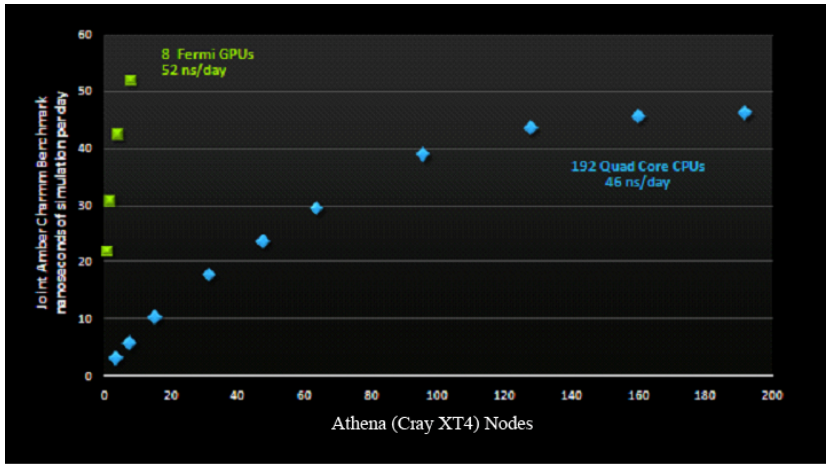
- 500 α-CD molecules
- 28000 molecules of 4MP
- 6000 water molecules
- ~(170 Å)$^3$ box
- Improved forcefield description

➡ **479000 atoms**

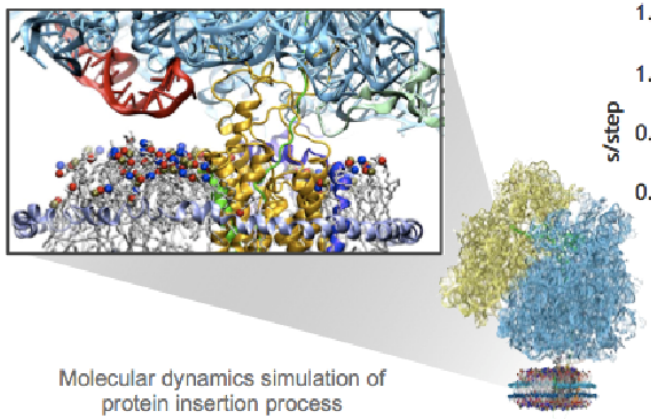


# Million atoms simulation

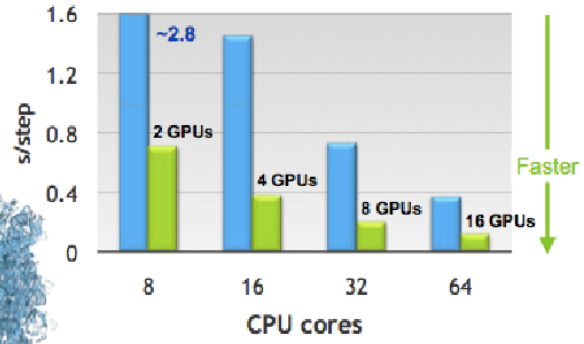



Amber GPU performance compared with that on Kracken@ORNL

Molecular dynamics simulation of protein insertion process




NCSA Lincoln Cluster performance
(8 Intel cores and 2 NVIDIA Tesla GPUs per node, 1 million atoms)

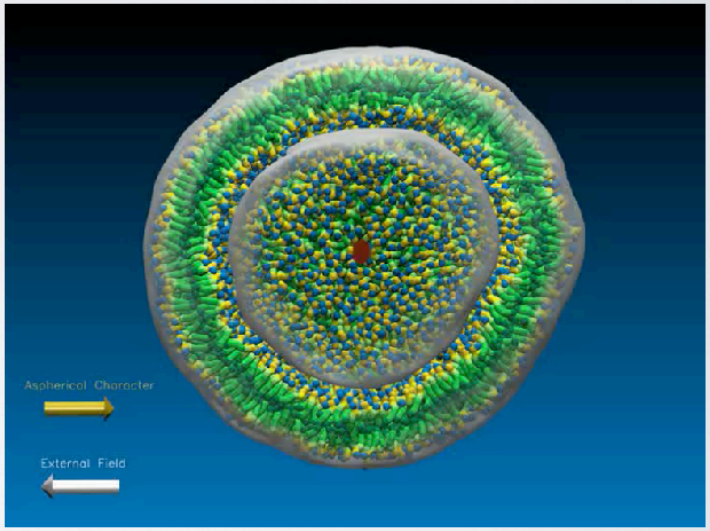
GPUs reduced time for simulation from **two months to two weeks!**

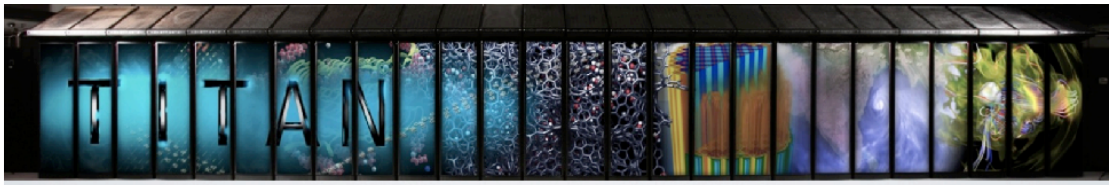
# Membrane Fusion

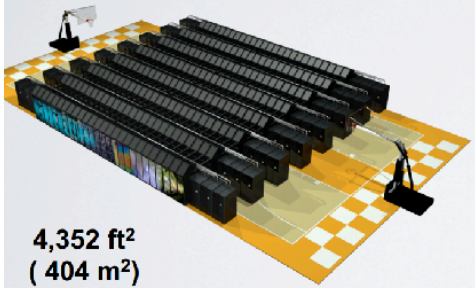
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

- Membrane fusion, which involves the merging of two biological membranes in a controlled manner, is an integral part of the normal life cycle of all living organisms.
- Viruses responsible for human disease employ membrane fusion as an essential part of their reproduction cycle.
- Membrane fusion is a critical step in the function of the nervous system
- Correct fusion dynamics requires realistic system sizes

39M Particle Liposome System2.7X Faster than 900 XK6 w/out Accelerators

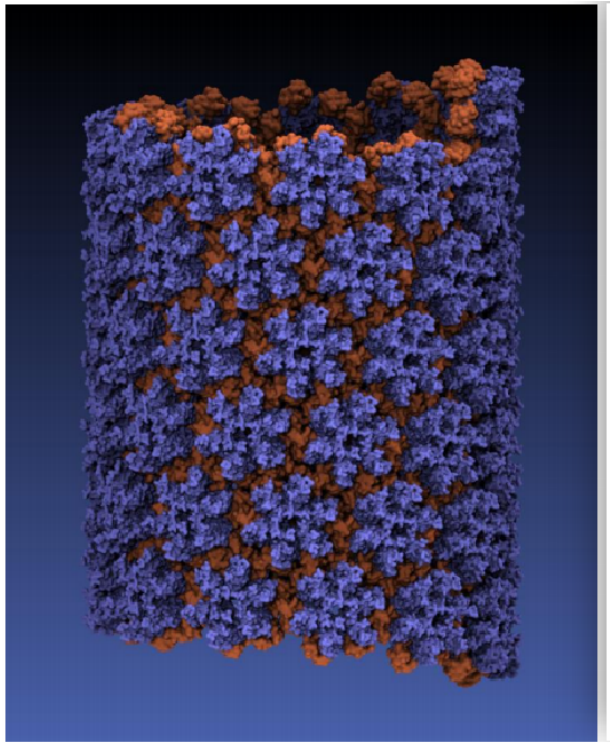


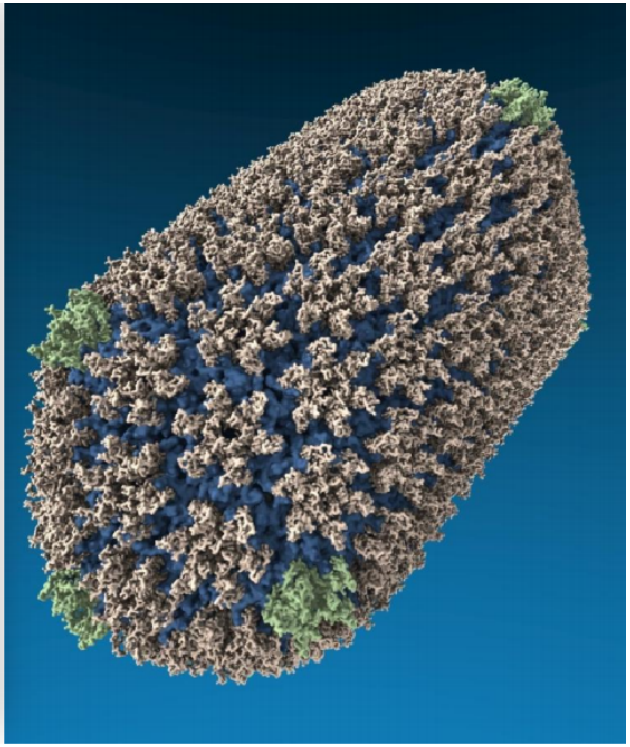




**SYSTEM SPECIFICATIONS:**
- Peak performance of 27.1 PF
  - 24.5 GPU + 2.6 CPU
- 18,688 Compute Nodes each with:
  - 16-Core AMD Opteron CPU
  - NVIDIA Tesla "K20x" GPU
  - 32 + 6 GB memory
- 512 Service and I/O nodes
- 200 Cabinets
- 710 TB total system memory
- Cray Gemini 3D Torus Interconnect
- 8.9 MW peak power

# All atom HIV Capsid Simulation



**Up to 64M atoms on Blue Waters, VMD "Quick Surf" Representation, Ray Tracing**

http://www.ncsa.illinois.edu/enabling/bluewaters http://www.ks.uiuc.edu/Research/vmd/

# Running AMBER on GRID

Giulio Rastelli and col. from University of Modena deployed initially AMBER on GRID.

Contacts were established with the institution distributing Amber regarding the license policy on the grid.

The outcome of the negotiation was that we were allowed to deploy Amber on the grid under the following conditions*:

- Each cluster deploying Amber had to have at least one license.
- Grid users allowed to use Amber had to come from one of the laboratories owning an Amber license.
- Grid users allowed to use Amber under the conditions described above could deploy their computations on all the grid clusters.


https://www.wenmr.eu/wenmr/resources/service/amber-web-portal

I. Bertini et al., **A Grid-enabled web portal for NMR structure refinement with AMBER**, Bioinformatics, 27(17), 2348 (2011)

•Vincent Breton, Doman Kim, and Giulio Rastelli, WISDOM: A Grid-Enabled Drug Discovery Initiative against Malaria, in Grid Computing: Infrastructure, Service and Applications, Di Lizhe Wang,Wei Jie,Jinjun Chen, pp. 373

# To know more about it

- Freezing on heating of liquid solutions, M. Plazanet, C. Floare, M.R. Johnson, R. Schweins, H.P. Trommsdorff, J. Chem. Phys. 121 (2004) 5031
- J. Chem. Phys. 125 (2005) 154504
- Chem. Phys. 317 (2006) 153
- Chem. Phys. 331 (2006) 35
- J. Phys. Cond. Mat. 19 (2007) 205108
- Phys. Chem. Chem. Phys. 12 (2010) 7026

# OF NOTE

EARTH SCIENCE

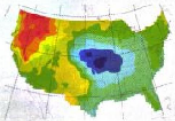
## Extra rainfall may stem warming in Midwest

Predicted increases in rain in parts of the Midwest may reduce the temperature effect that scientists expect from global warming during the next few decades.

Computer simulations of the climate in the lower 48 United States suggest that if atmospheric concentrations of planet-warming carbon dioxide rise about 1 percent per year, the average temperature across the region will be about 3°C hotter in the 2040s than it was in the 1990s, says Zaitao Pan, a climatologist at St. Louis University.

The climate models also suggest that low-altitude winds that bring moist air from the Gulf of Mexico to the Great Plains will be stronger in summer months in the 2040s than they were in the 1990s. That will boost Midwest precipitation by as much as 1 millimeter per day over the measured daily averages a decade ago, says Pan. Evaporation of the extra moisture will consume solar energy that otherwise would have warmed the region's air. All told, summertime temperatures in some parts of the Midwest might end up only 0.5°C warmer in the 2040s than they were in the 1990s.

Any extra evaporative cooling in the Midwest might be a temporary phenomenon, warn Pan and his colleagues in the Sept. 16 *Geophysical Research Letters*. As global warming becomes more severe beyond the 2040s, the region might not continue to receive the palliative precipitation. —S.P.



**COOL SPOT** Temperatures in portions of the Midwest may increase only 0.5 to 1.0°C (dark blue zones) during the next half century because of increased rainfall.

PHYSICS

## To freeze this liquid, add heat

Researchers in France have discovered a liquid mixture that freezes into a waxy crystalline solid when heated. It appears to be the first solution to exhibit an abnormal heat-induced transition from liquid to solid rather than the other way around, report Hans-Peter Trommsdorff of Joseph Fourier University in Grenoble and his colleagues. They detail the finding in the Sept. 15 *Journal of Chemical Physics*.

The scientists created the surprising substance by mixing alpha-cyclodextrine—whose molecules are loops made of six glucose molecules—with water and the common, foul-smelling organic solvent 4-methylpyridine.

At room temperature, about 20°C, the mixture is a clear liquid. It transforms into a milky white block at a temperature between 45°C and 75°C, depending on the proportions of the mixture's ingredients. This is not a gelling effect, the researchers say.

"There's no chemical change," notes physical chemist Ralf Schweins of the Laue-Langevin Institute in Grenoble, a member of the research team. "When you cool it down, it becomes a liquid again." Tests also indicate that the heat-formed solid reliquefies when heated above approximately 95°C, the team reports.

The team's computer simulations suggest why solidification occurs at the transition from cooler liquid to warmer solid. Some weak intermolecular attractions, called hydrogen bonds, which ordinarily would strengthen links between the glucose components of alpha-cyclodextrine become disrupted. This allows new hydrogen bonds to form between the solution's different constituents. —P.W.

ASTRONOMY

## Martian water everywhere

Mars once had an ocean at least a half-kilometer deep and larger than the combined area of all five Great Lakes on Earth. That's the conclusion of researchers who have analyzed data collected by orbiting spacecraft as well as the Mars rover Opportunity.

Last March, Opportunity found at its Meridiani Planum landing site rocks containing sulfates, which could have been created only in the presence of water (*SN: 3/6/04, p. 147*). The sulfates occurred in an outcrop of light-colored rock.

Bryan M. Hynek of the University of Colorado in Boulder then compared infrared and visible-light images of those rocks with images of light-toned outcrops extending hundreds of kilometers to the north, east, and west. The colors of the distant rocks, recorded by the orbiters Mars Global Surveyor and Mars Odyssey, match the signature of sulfates examined by the rover. "I see evidence for this [water-related] process over a large area," says Hynek, who describes his findings in the Sept. 9 *Nature*.

In the August *Journal of Geophysical Research*, Philip R. Christensen and Steven W. Ruff of Arizona State University in Tempe also argue for a large ocean in the past of Meridiani Planum, on the basis of data the two orbiters gathered before Opportunity reached Mars.

A spectrometer aboard the European Space Agency's Mars Express spacecraft has also recently identified sulfates in the far-flung rocks. Jean-Pierre Bibring of the Institute of Spatial Astrophysics in Orsay, France, presented the findings in late September at the International Mars Conference in Ischia, Italy. —R.C.

NEUROSCIENCE

## Verbal sighting in brains of the blind

Brain areas that typically play a key role in vision instead contribute to language skills among blind people, a new study finds. This observation underscores the brain's ability to adapt to individual circumstances, say Leonardo G. Cohen of the National Institute of Neurological Disorders and Stroke in Bethesda, Md., and his colleagues.

The scientists administered a verbal task to nine adults with normal sight and nine adults who had lost their sight by age 4. Each volunteer listened to a series of spoken nouns, such as *apple*, and had 5 seconds after each one to say an appropriate verb, such as *eat*.

In some trials, the researchers temporarily disabled various brain regions by briefly transmitting focused magnetic pulses through the volunteers' skulls. Only blind volunteers made a large number of mistakes on the verbal task—such as responding to *apple* with *jump*—when the pulses disabled either of two rear-brain regions. In sighted individuals, these structures participate in early stages of visual processing.

Sighted participants erred frequently on the task only after the magnetic pulses temporarily sidelined a frontal-brain area previously implicated in verbal skills. Pulses to that area didn't affect the blind volunteers, the researchers report in the November *Nature Neuroscience*. —S.B.





## Law-breaking liquid defies the rules

29 September 2004

**Physicists in France have discovered a liquid that "freezes" when it is heated. Marie Plazanet and colleagues at the Université Joseph Fourier and the Institut Laue-Langevin, both in Grenoble, found that a simple solution composed of two organic compounds becomes a solid when it is heated to temperatures between 45 and 75 °C, and becomes a liquid when cooled again. The team says that hydrogen bonds are responsible for this novel behaviour (M Plazanet *et al.* 2004 *J. Chem. Phys.* 121 5031).**

Solids usually melt when they are heated, and liquids turn into gas, although exceptions do exist when heating leads to chemical changes that cannot be reversed, such as polymerisation. However, a reversible transition in which a liquid becomes a solid when heated has never been observed until now.

Plazanet and colleagues prepared a liquid solution containing α-cyclodextrine (αCD), water and 4-methylpyridine (4MP). Cyclodextrines are cyclic structures containing hydroxyl end groups that can form hydrogen bonds with either the 4MP or water molecules.

At room temperature, up to 300 grams of αCD can be dissolved in a litre of 4MP. The resulting solution is homogenous and transparent, but it becomes a milky-white solid when heated. The temperature at which it becomes a solid falls as the concentration of αCD increases.

Neutron-scattering studies revealed that the solid phase is a "sol-gel" system in which the formation of hydrogen bonds between the αCD and the 4MP leads to an ordered, rigid structure. At lower temperatures, however, the hydrogen bonds tend to break and reform within the αCD, which results in the solution becoming a liquid again.

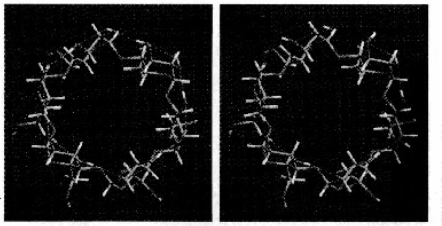
Molecular dynamics simulations by Plazanet and co-workers confirmed that the cyclodextrine ring becomes distorted as it is heated up to close to the solidification temperature. The hydrogen bonds within the αCD break and the hydroxyl groups rotate towards the outside, which allows a network of bonds to form between the different molecules. The team has found a number of cyclodextrine/pyridine systems that also become solid when heated, and is now looking more closely at the structure of the sol-gel system to understand the solidification mechanism in more detail.

About the author

Belle Dumé is Science Writer at *PhysicsWeb*

# Law-breaking liquid defies the rules

When you place a pan of water on a stove and turn up the heat, the last thing you expect to appear is ice. However, researchers in France have discovered a liquid that "freezes" when it is heated. Marie Plazanet and colleagues at the Université Joseph Fourier and the Institut Laue-Langevin, both in Grenoble, found that a simple solution composed of two organic compounds becomes a solid when it is heated to temperatures between 45 and 75 °C. Moreover, the solidified solution becomes a liquid again when it is cooled (*J. Chem. Phys.* **121** 5031).



Breaking bonds – hydrogen bonds (yellow) in the cyclodextrine molecule are thought to be responsible for causing a solution of the molecules to freeze when it is heated.

Thermodynamics tells us that the entropy of a system increases when the temperature rises, which means that solids usually melt when they are heated, while liquids turn into gas. There are some exceptions to this rule. For example, heating can lead to chemical changes that cannot be reversed, such as polymerization, and quantum fluids such as helium-3 also exhibit counterintuitive phase changes. But a reversible transition in which a simple molecular liquid becomes a solid when heated has never been observed at room temperature until now.

Plazanet and colleagues prepared a liquid solution containing α-cyclodextrine (αCD), water and 4-methylpyridine (4MP). At room temperature, up to 300 g of αCD can be dissolved in a litre of 4MP, which results in a homogenous and transparent solution. When it is heated, the solution forms a milky-white solid, and the temperature at which this takes place decreases as the concentration of αCD increases.

Neutron-scattering studies reveal that the solid phase is a "sol-gel" system in which the formation of hydrogen bonds between the αCD and the 4MP leads to an ordered, rigid structure. At lower temperatures, however, the hydrogen bonds tend to break and reform within the αCD, causing the solution to become a liquid again.

The Grenoble team attributes this novel behaviour to the hydrogen bonds, and is now trying to understand the solidification mechanism in more detail. Molecular-dynamics simulations confirm that the αCD ring becomes distorted as it is heated to close to the solidification temperature. As a result, the hydrogen bonds within the αCD break and the hydroxyl groups rotate towards the outside, allowing a network of bonds to form between the different molecules.

# Other references

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  - http://bit.ly/cfloareILL2004
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ISERE

Le Dauphiné liberé, 26 Avril 2005

# L'énigme du cristal fondant

**GRENOBLE.** Il durcit quand on le chauffe. Il devient liquide quand on le refroidit. Une équipe de l'ILL et de Joseph-Fourier cherchent une explication

Marie, Mark et Peter, et, sur l'écran, les deux tubes soumis ou non à la flamme : d'un côté, la solution durcit à la chaleur, de l'autre, elle redevient liquide.

L'affaire se résume finalement à cela, à un bien étrange phénomène : voilà un cristal très versatile, qui fond quand on le refroidit, et qui "gèle" lorsqu'on le chauffe !

De quoi faire sursauter les équipes communes de l'Institut Laue Langevin (ILL) et de l'Université Joseph-Fourier, qui se grattent la tête en observant les contenus des deux éprouvettes de test. A l'ILL, Marie Plazanet, Mark Johnson et Peter Trommsdorf reprennent l'histoire à l'origine : "Un de nos thésards nous a confié son souci ; il souhaitait étudier le comportement d'une molécule en l'incluant dans une cage moléculaire. Une manipulation classique pour nous, qui passe par une évaporation, pour mettre l'ensemble en évidence. Une journée après, toujours pas d'évaporation. Nous lui avons conseillé de chauffer le tout, histoire d'accélérer le processus. Las, il n'en sortait plus : sa solution s'était solidifiée. Puis, en se refroidissant, elle est redevenue liquide ! "

Voilà de quoi étonner. Parce qu'on a plus l'habitude de voir, sous l'action de la chaleur, un solide fondre ou un liquide se transformer en gaz ! Nos chercheurs ont donc immédiatement mis le nez sur la composition de cette solution dont on dira, pour faire simple, qu'elle est composée d'un mélange d'eau, d'alpha-cyclodextrine et de 4-méthylpyridine. En la chauffant entre 45 et 75° centigrades, il se pourrait que les liaisons d'hydrogène se rompent et les molécules "s'ouvrent", ce qui leur permettrait de faire une jonction, de l'une à l'autre. D'où cette "solidification" pour le moins surprenante.

Et alors ? "Alors, expliquent Marie, Mark et Peter, nous cherchons à mieux comprendre le mécanisme de solidification, l'arrangement particulier des molécules. Ensuite, nous avancerons, progressivement. "

Pour ce faire, ils profitent bien entendu de la source à neutrons de l'ILL, mais également du rayonnement synchrotron de l'accélérateur voisin, de l'European Synchrotron Radiation Facility. Tout en s'étonnant de l'agitation du milieu scientifique provoquée par cette découverte. "Celle-ci ne date pas d'hier. Mais le temps que nous publiions l'information, comme il se doit, et l'information a été rapidement reprise sur le Web, nous avons été sollicités de toutes parts. "

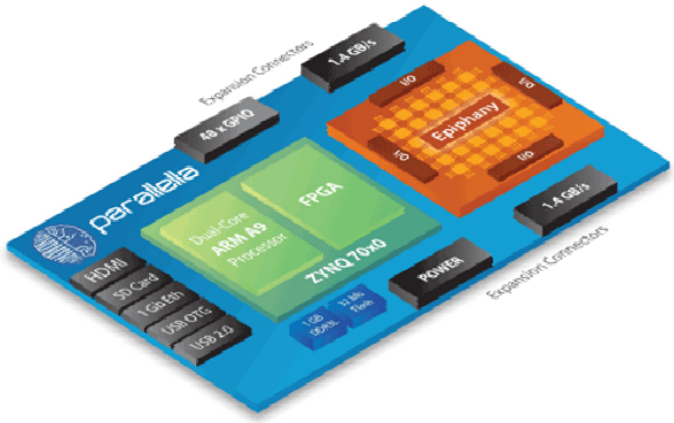
## Un avenir dans les cosmétiques ?

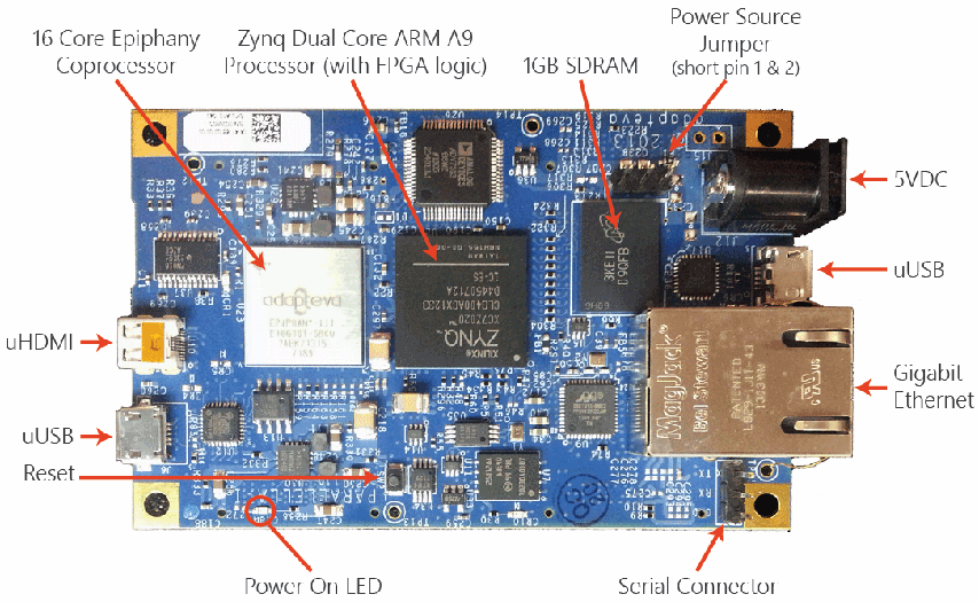
Alors quelles applications possibles pour ce "cristal" si changeant ? Elles pourraient se situer dans les carburants, dans la mécanique, dans la micro et la nano-électronique. Et, en y réfléchissant, cette faculté de passer aisément d'un état à l'autre pourrait même se révéler très précieuse pour les produits cosmétiques !

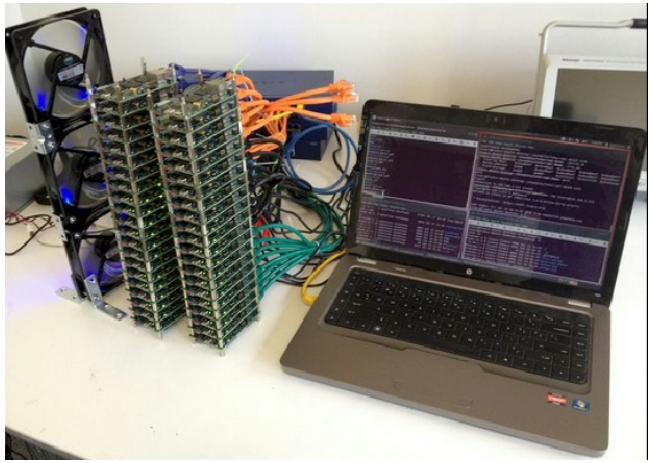
**Olivier PENTIER**

# Future Architectures - Adapteva Parallella

- Claimed to be the world most efficient computer
- Epiphany III - 16 RISC cores, 32 GFLOSP peak performance
- Epiphany IV - 64 RISC cores, 100 GFLOSP peak performance
- less than 2W max power
- Scalable to 4096 cores on a single chip
- 70 GFLOPS/W in 28 nm LP process
- Starting at 99$



A 42-node cluster of Parallella-16 boards from Adapteva

http://www.adapteva.com http://www.parallella.org

# Yocto Project

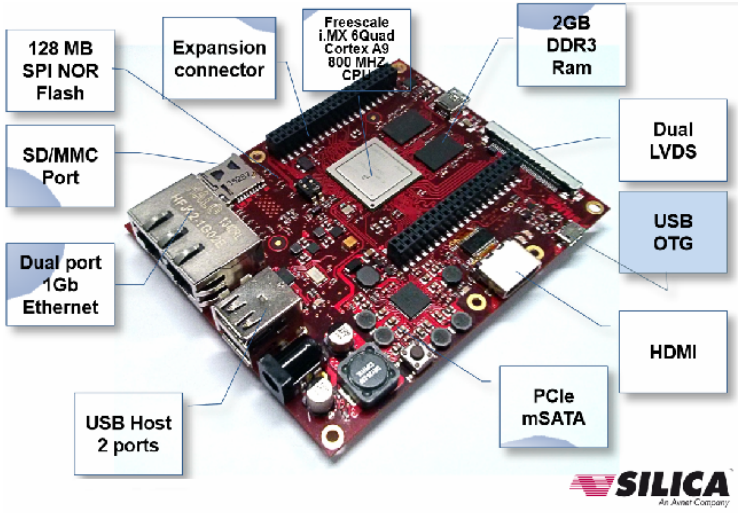
- It's not an embedded Linux distribution – it creates a custom one for you
- The Yocto Project is an open source collaboration project that provides templates, tools and methods to help you create custom Linux-based systems for embedded products regardless of the hardware architecture

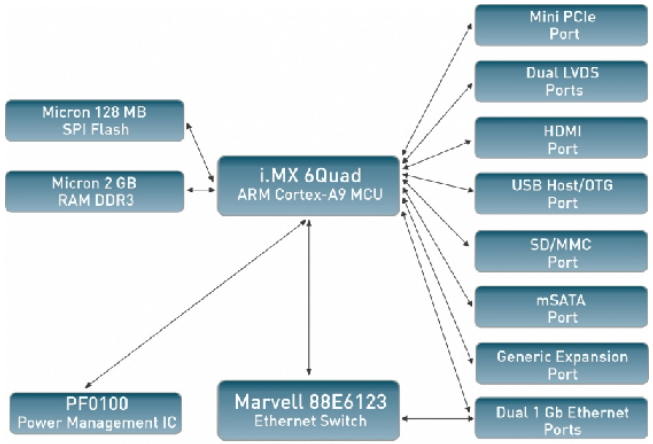
Andrew Feldman, GM and corporate VP at AMD, Jun. 2013:

The data center is changing and ARM will be the compute

## Silica Architech Tibidado Board

- Freescale i.MX 6Quad - 4 x ARM Cortex-A9 @ 1.2 GHz per core, 1 MB L2 cache
- GPU 3D graphics: Vivante GC2000; 2D graphics engines: GC355 (Vector), GC320 (Composition)
- 2GB DDR3 RAM …




http://www.yoctoproject.com http://www.architechboards.org

# Intel To Offer Custom Xeons With Embedded FPGAs

Intel is going to start embedding custom FPGAs into its own CPU silicon

*"To ensure that ARM or other alternative architectures don't gain ground in the data center, Intel is launching a customizable chip that marries its Xeon CPUs with an FPGA.", Gigaom Structure conference, Jun. 18, 2014*

http://bit.ly/IntelCustomizableChip

Diane Bryant, SVP and General Manger of Intel's data center group & Tom Krazit

- Intel will build a customizable and programmable CPU that combines an Intel processor and a programmable chip from an undisclosed partner. Will be Altera or Achronix ? Altera is a safe bet.
- "using FPGAs to accelerate certain specific types of workloads, Intel Xeon customers can reap higher performance for critical functions without translating the majority of their code to OpenCL or bothering to update it for GPGPU.", HotHardware
- Probably they are already used by Microsoft in Project Catapult to process Bing queries at a faster rate, Doug Burger, Wired


http://www.wired.com/2014/06/microsoft-fpga/

# A great tool for developers

- Vagrant is an amazing tool for managing virtual machines via a simple to use command line interface. With a simple vagrant up you can be working in a clean environment based on a standard template.

```
$ vagrant box add {title} {url}
$ vagrant init {title}
$ vagrant up
```

The list of boxes was last updated on May 20th, 2014.

| Name | Provider | URL | Size |
|---|---|---|---|
| Debian 7.3.0 64-bit Puppet 3.4.1 (Vagrant 1.4.0) | VirtualBox 4.3.6 | Copy https://dl.dropboxusercontent.com/u/29173092/vagrant-boxes/debian7.3.0-vbox4.3.6-puppet3.4.1.box | 682MB |
| OpenBSD 5.4 64-bit + Chef 11.8.2 (150GB HDD) | VirtualBox | Copy http://vagrant.inagile.org/vagrant-obsd54-amd64.box | 1000MB |
| OpenBSD 5.3 64-bit (Vagrant 1.2) | VirtualBox | Copy https://dl.dropboxusercontent.com/u/12089300/VirtualBox/openbsd53_amd64_vagrant12.box | 296MB |
| OpenBSD 5.3 64-bit | VirtualBox | Copy https://dl.dropboxusercontent.com/u/12089300/VirtualBox/openbsd53_amd64.box | 303MB |
| Aegir-up Aegir (Debian Squeeze 6.0.4 64-bit) | VirtualBox | Copy http://ergonlogic.com/files/boxes/aegir-current.box | 297MB |
| Aegir-up Debian (Debian Squeeze 6.0.4 64-bit) | VirtualBox | Copy http://ergonlogic.com/files/boxes/debian-current.box | 283MB |
| Aegir-up LAMP (Debian Squeeze 6.0.4 64-bit) | VirtualBox | Copy http://ergonlogic.com/files/boxes/debian-LAMP-current.box | 388MB |
| AppScale 1.12.0 (Ubuntu Precise 12.04 64-bit) | VirtualBox | Copy http://download.appscale.com/download/AppScale%201.12.0%20VirtualBox%20Image | 1900 MB |
| Arch Linux 64 (2014-06-20) | VirtualBox | Copy http://www.eduardoheredia.com.br/rep/vagrant/archlinux64.box | 292MB |
| Arch Linux 64 (2013-08-01) | VirtualBox | Copy https://dl.dropboxusercontent.com/u/31112574/arch64-20130801.box | 578MB |
| Arch Linux x86_64 (2013-08) | VirtualBox | Copy https://googledrive.com/host/0B_BLFE4aPn5zUVpyaHdLanVnMTg/vagrant-archlinux-2013-8.box | 394MB |
| Arch Linux 64 (2013-07-28) (Puppet and Chef installed) | VirtualBox | Copy https://dl.dropboxusercontent.com/u/9213047/arch64_2013_07_28.box | 533MB |
| Arch Linux 64 (2013-12-21) - Base Install | VirtualBox | Copy https://dl.dropboxusercontent.com/s/kp4m59j4k5ifj9l/vagrant-archlinux64-20131221.box | 405MB |
| Arch Linux 64 (2013-07-26) - Base Install | VirtualBox | Copy http://iweb.dl.sourceforge.net/project/flowboard-vagrant-boxes/arch64-2013-07-26-minimal.box | 433.2 MB |
| Arch Linux 64 (2013-07-26) - Chef 11.6.0 from gem, Ruby from pacman | VirtualBox | Copy http://iweb.dl.sourceforge.net/project/flowboard-vagrant-boxes/arch64-2013-07-26-chef.box | 466.7 MB |

http://vagrantup.com http://vagrantbox.es

# Grid Training Tool

Gridseed

- Gridseed – A Virtual Training Grid Infrastructure
  - a fully fledged Grid infrastructure based on the gLite middleware
  - developed to easily deploy a training grid infrastructure
  - consists of VirtualBox virtual machines, each of them running one or more gLite services
  - unfortunately not updated, last version 1.6.2 (13th December 2010)

and other tools:

- Milu (Miramare Interoperable Lite User Interface) a tool to set up easily an UI on (almost) any machine (https://eforge.escience-lab.org/gf/project/milu/)
- EPICO – eLab Procedure for Installation and Configuration (http://epico.escience-lab.org/)
- BEMuSE: Bias-Exchange Metadynamics Submission Environment (https://euindia.ictp.it/bemuse/)

Thank you for your attention