

Some Aspects of Supercomputing in Hungary

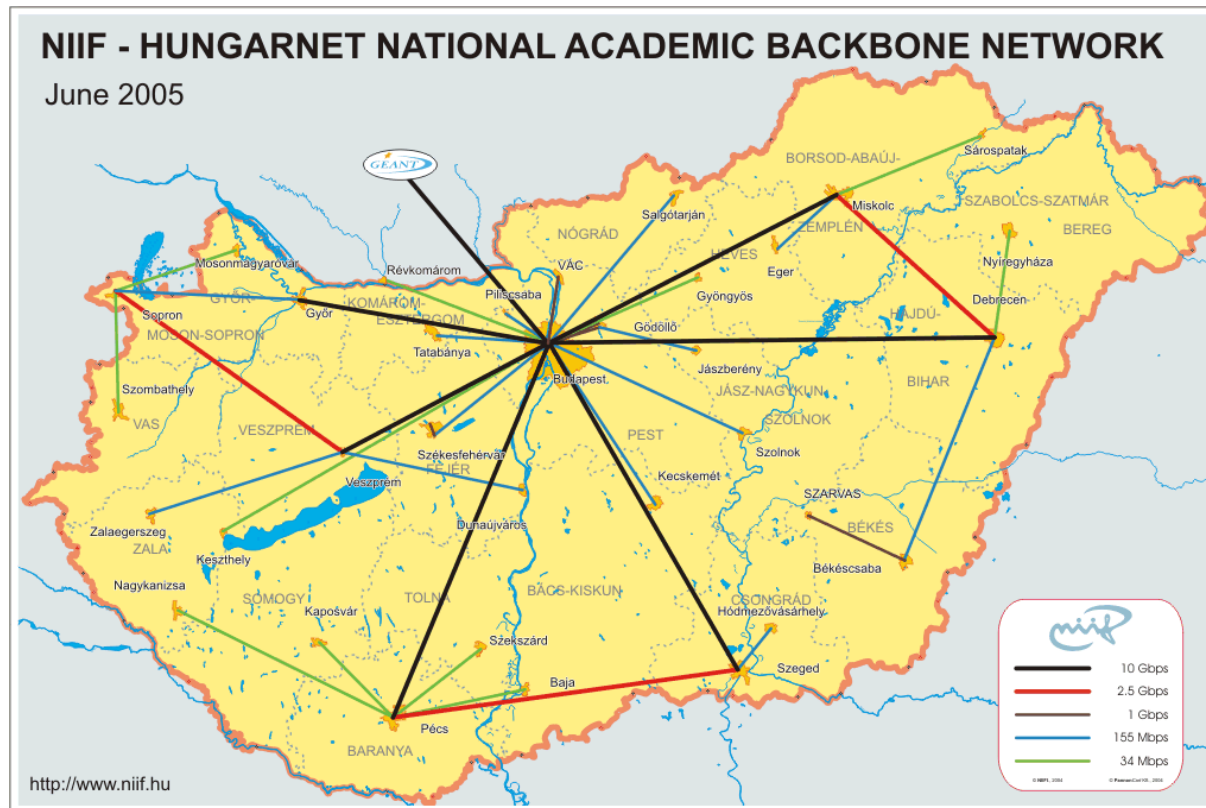
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WS Jülich, January 15-16, 2006

Apologies...

Centers of Higher Education and Research in Hungary



Budapest

see next slide

Univ. Debrecen

Univ. Szeged

Univ. Pécs

Univ. Miskolc

Univ. Veszprém

Győr, Sopron,
Kaposvár...

Research Institutes of the Hungarian Academy of Sciences:

Debrecen: Institute for Nuclear Research (ATOMKI)

Szeged: Center for Biological Research (BKI)

Budapest and surrounding:

Higher Education

Eötvös University

Budapest University of Technology and Economics (BME)

Semmelweis University

Corvinus University

St. Steven University (Gödöllő)

Pázmány Catholic University (Pomáz)

Four „universities” of music, art, appl. art, theatre and movies

Several „Technische Hochschulen”

Research Institutes of the HAS

Inst. for High Energy Physics (RMKI)

Inst. for Solid State and Optics (SZFKI)

Inst. for Technical Physics and Material Science (MFA)

Inst. for Nuclear Energy (AEKI)

Center for Research in Chemical (KKK)

Inst. for Computation and Automatization (SZTAKI)

Konkoly Thege Institute for Astronomy

National Office for Development of Computational Infrastructure

→ (NIIF)

Supercomputing in Hungary

- Supercomputing facilities are available in Hungary for basic research at **NIF** as service to the community (see presentation by Dr. Máray) and at some universities (**Eötvös, BME**). At Eötvös: „Poor man’s supercomputer” **PMSC** → Wuppertal (Prof. Fodor)
- Further facilities are e.g. at the National Service for **Meteorology** (outside not yet available)
- There is a generally distributed view that the future of SC is **GRID** (see Dr. Máray). The knowledge about top performance computers is rather limited. This restricts the choice of problems considered for solution, as this choice is usually conditioned by the available tools.
- There is no generally accepted definition of SC. Some consider calculation on a 20 processor **PC cluster** under a simple protocol as SC.
- Most of the SC in Hungary is part of international collaborations where SC facilities are often provided by or through the **foreign partner**.

- 2005 the NIF machine was used for 53 projects resulting in an, with, e.g., 87% usage December 2005
- Main areas of supercomputing carried out in Hungary
 - Calculation of electronic structure in molecules and solid state materials (NIF)
 - Astrophysics (NIF)
 - Simulations related to nuclear reactors (NIF)
 - Geophysics (Evaluation of satellite provided data) (NIF)
 - Medical research (simulation of enzyme functioning mechanisms (NIF))

 - High energy physics (not at NIF, theor: „PMSC”, exp: GRID)
 - Many body model simulations (mostly PC clusters)

 - Engineering design (very little)
 - Math and computing (very little)

Questionnaire

1. Name of the project leader:
2. Title of the project, duration
3. Supercomputer used; peculiarities (e.g., number of processors, speed etc.)
4. Supercomputing CPU time needed
5. Computing specialties (parallel, vector etc.)
6. Important results, publications
7. Remarks

Some examples

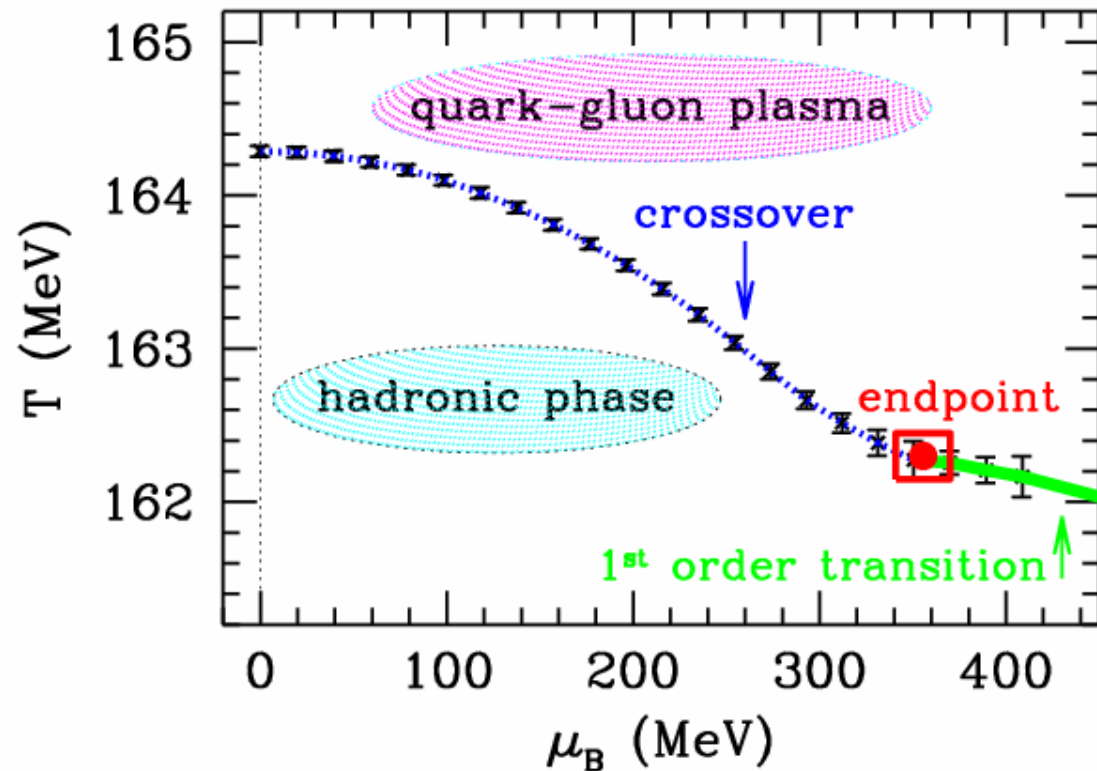
1. Lattice QCD (Z. Fodor, S. Katz, F. Csikor, Eötvös)

„Poor man’s supercomputer”, PC clusters with next neighbor gigabit communication.

1.5 Gflops/processor sustained speed is reached.

350 nodes * 1.5 Gflops/node * 4 years = 2.1 Tflop-years

QCD phase diagram



2. Electronic structure of molecules

(A.G. Császár, Eötvös)

Memory need: ~ 100 Gbyte, Disk: ~Tbyte

Partly parallelizable program, > 64 procs

-- „Ab initio” thermochemistry

-- Structure of biomolecules

-- Rovibrational spectrum of small molecules

E.g. ab initio calculation for water (Science 2003):

Including relativistic effects, nuclear motion (non-adiabatic effects), etc.

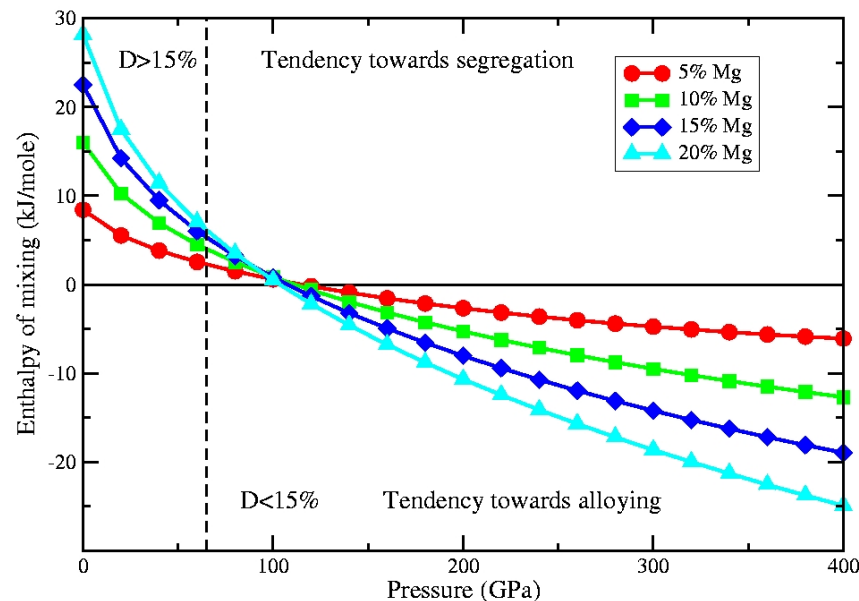
Order of magnitude improvement as compared to earlier results.

(See other results of the same group in Prof. Szalay’s presentation)

3. Electronic structure calculations (J. Kollár, L. Vitos, SZFKI)

SUN 15000, 128 procs

- Computational study of the tribological properties of metals
- Beating the Miscibility Barrier between Iron Group Elements and Magnesium by High-Pressure Alloying



PRL Dec. 2005 cover

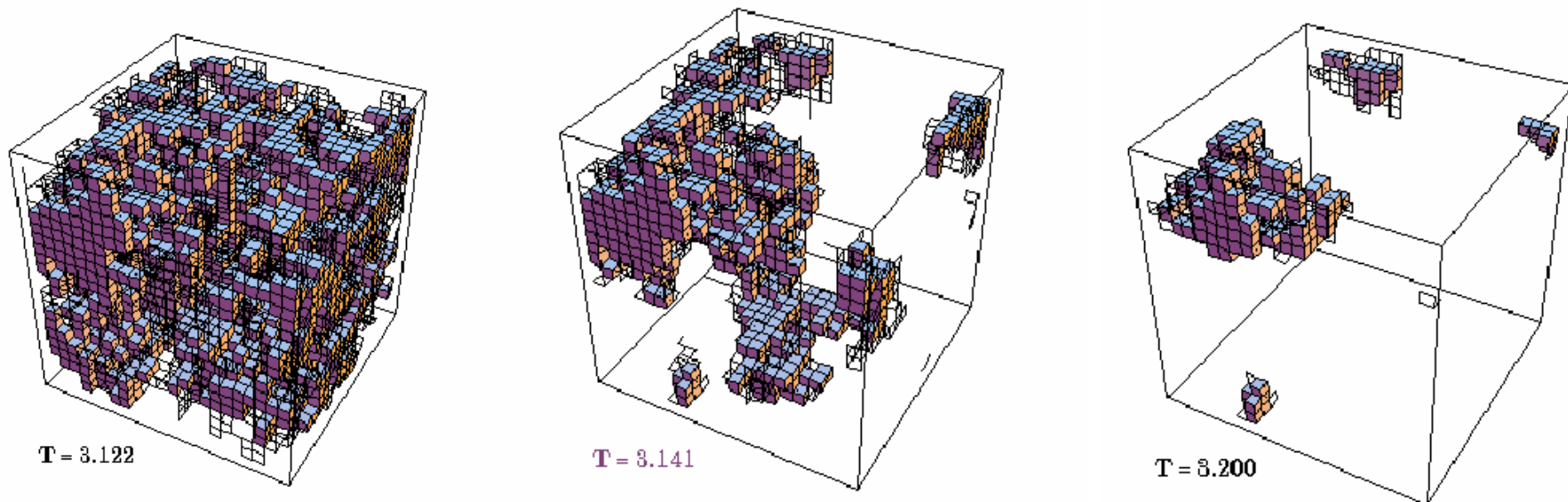
(For other calculations in solid state physics see Dr. Udvardi's presentation)

4. Dynamics of nonequilibrium and random systems (F. Iglói, P. Lajkó, R. Juhász, SZFKI)

PC cluster > 20 procs, CPU time > 60 000hours/year

Many systems investigated

E.g.: Large q -state Potts model in 3d: Strong enough
Disorder makes the transition 2nd order (Europhys. Lett. 2005)

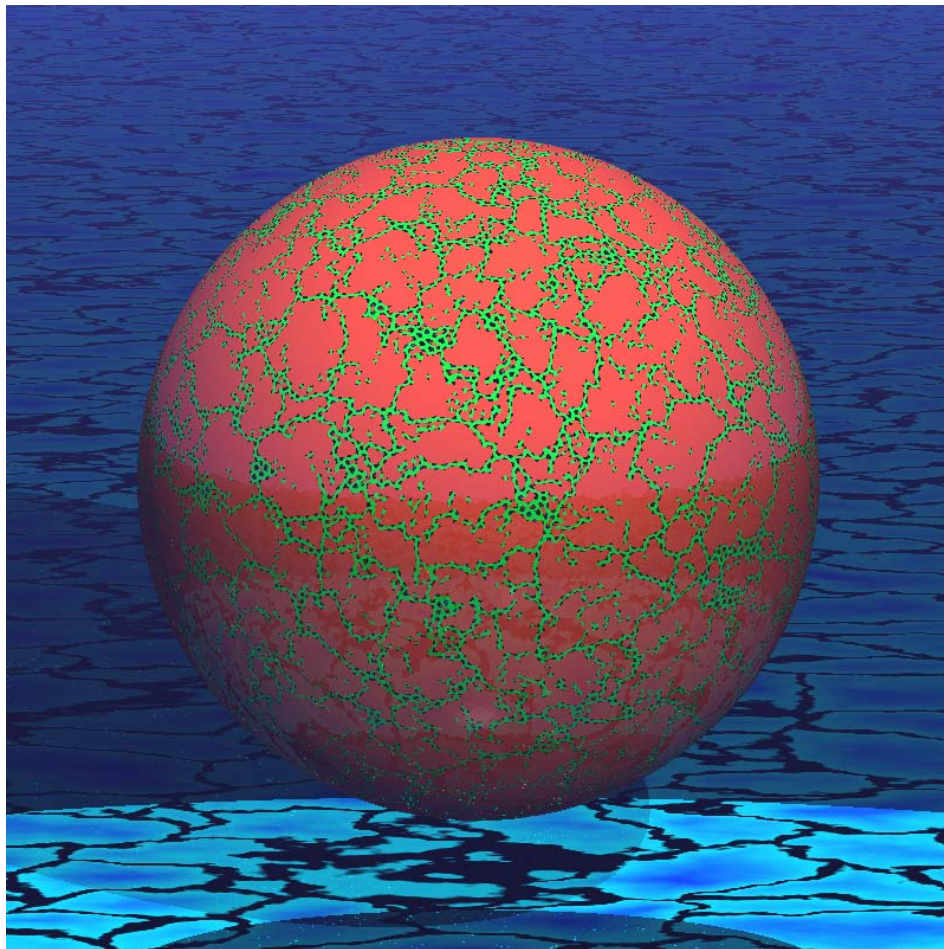


5. Statistical physics simulations (F. Kun, K.F. Pál, I. Varga, Debrecen)

>1400 hours/year on PC clusters of 32 procs

-- Structure formation in dipolar monolayers

-- Fracture and fragmentation of solids

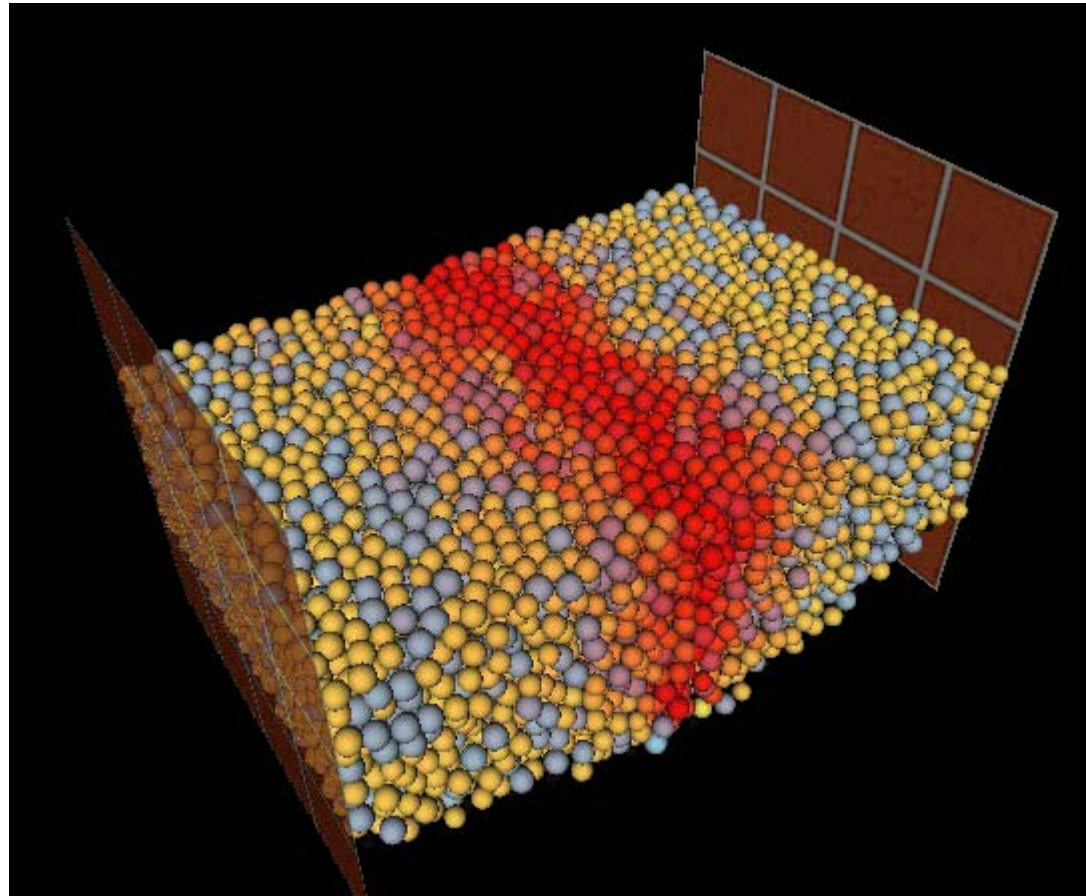


Explosion of a spherical shell. The rupture lines were projected back

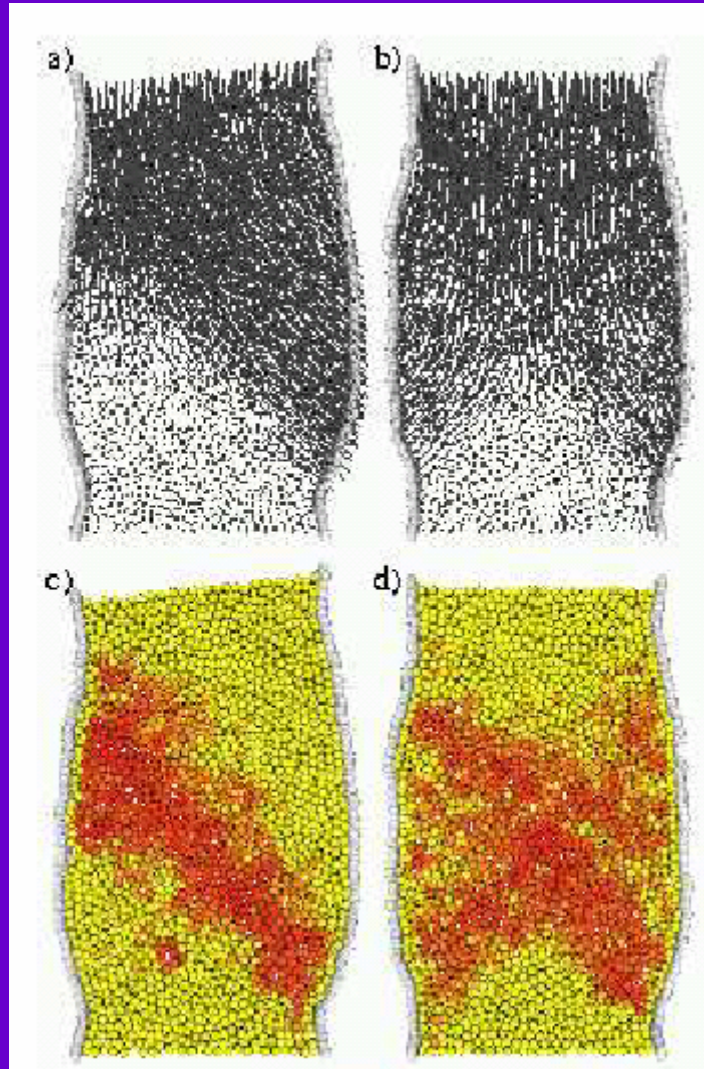
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6. Granular systems (J. Kertész, T. Unger, J. Török, S. Fazekas, BME)

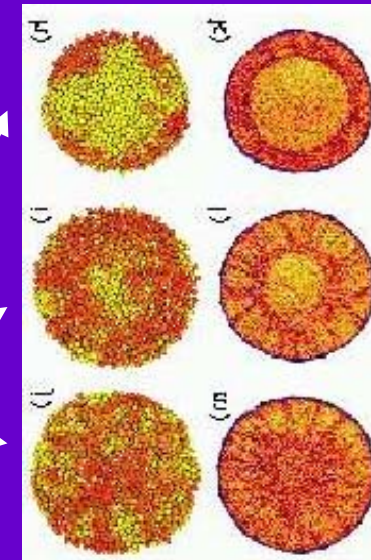
PC cluster of 48 procs, MD and CD techniques



Upper platen
can tilt



Upper platen
cannot tilt



Microgravity CT