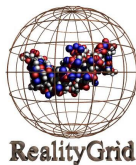


HPC in Modelling Complex Fluids

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- 1 Complex fluids
 - Amphiphile mesophases: an interesting class of complex fluid
- 2 What HPC makes possible
 - Simulation of complex fluids
- 3 The TeraGyroid project

What is a complex fluid?

A fluid in whose macroscopic flow is affected by its microscopic properties

Such as:

- beer

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Because they're fluids.

Fluids are hard to model in the first place; Navier-Stokes equations are nonlinear.

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Like a soap molecule

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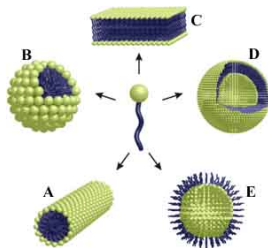


Image from <http://www.vcbio.sci.kun.nl/fesem/applets/amphiphiles/>

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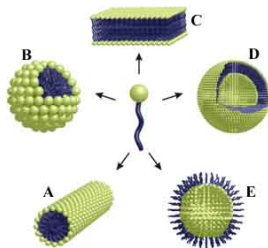


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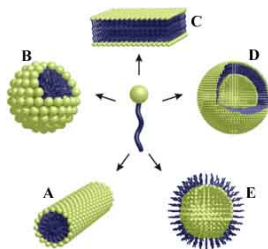


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Cubic mesophases

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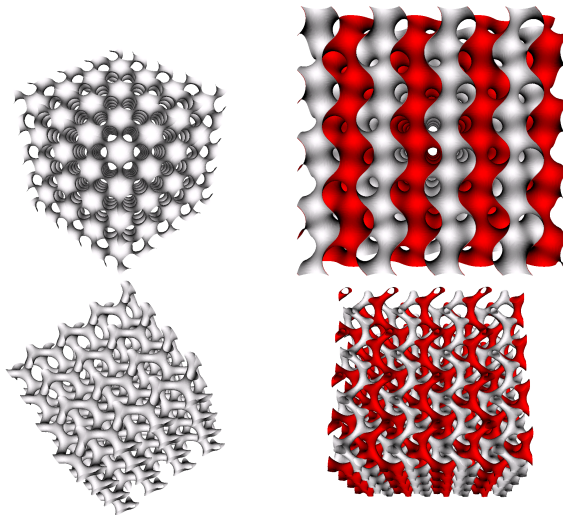
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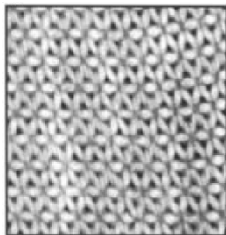
Cubic mesophases

- Amphiphile mixtures will often produce very strange-looking morphologies
- These will self-assemble from a random mixture!
- We've been using HPC to model a particular sort of cubic mesophase, the *gyroid*.

Geometry of the gyroid

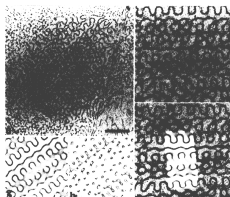


Gyroids in the real world



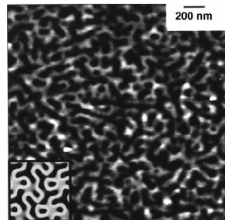
Gyroidic
copolymer melt

(Shefelbine et al., J. Am.
Chem. Soc. **121**, 8457 (1999))



Gyroid in
biological system

(Landh, FEBS Lett **369** 13-17
(1995))



Self-assembling
ceramic gyroid

(Chan et al., Science **286**:
1716-1719 (1999))

Self-assembly is hard to model.

Self-assembly dynamics are a typical complex fluid problem: interactions between macroscopic flow and microscopic properties are crucial.

HPC and complex fluids

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- Hence is called a mesoscale method

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- Largest system was 1024^3 over 2048 CPUs of `lemieux.psc.edu`

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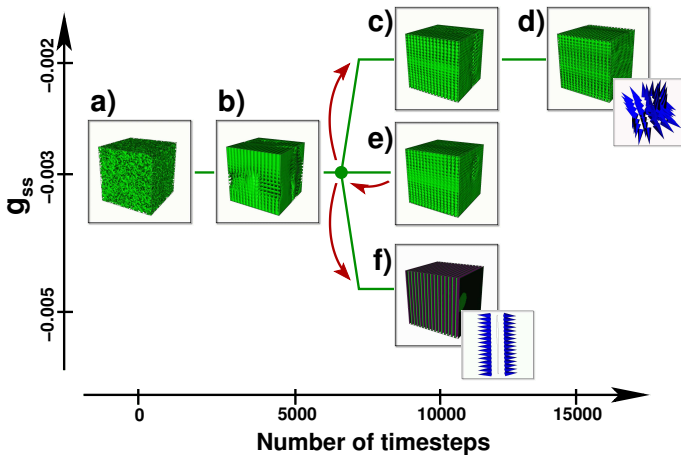
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- Also helps reduce storage requirements

Computational steering in action



Computational grids

- Link distributed resources through high-performance network

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- Use remote storage, compute, visualization facilities
- Use remote expertise: permits allows scientists in different countries to work together on the same simulation in real-time

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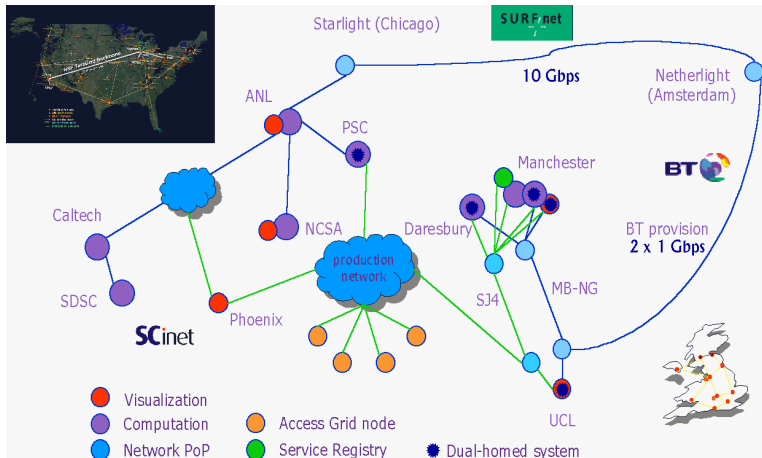
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- Won "Most innovative data-intensive application" at SC03

The TeraGyroid network



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- Migrate simulation from Manchester to NCSA

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- Viewed via multicast at UCL, BT Adastral Park, Boston, Phoenix, and SCGlobal sites

Hardware infrastructure

Computation

- HPCx (Daresbury), 1280 CPUs IBM Power4 Regatta, 6.6Tflops, 1.024TB
- Lemieux (PSC), 3000 procs HP/Compaq, 6Tflops peak, 3TB
- TeraGrid Itanium2 cluster (NCSA), 256 procs, 1.3Tflops peak
- TeraGrid Itanium2 cluster (SDSC), 256 procs, 1.3Tflops peak
- Green (CSAR), SGI Origin 3800, 512 cprocs, 0.512TB (shared)
- Newton (CSAR), SGI Altix 3700, 256 Itanium2 procs 384GB (shared)

Hardware infrastructure

Visualization

- Bezier (Manchester), SGI Onyx 300, 6x IR3, 32procs
- Dirac (UCL), SGI Onyx2, 2x IR3, 16 procs
- SGI loan machine (Phoenix), SGI Onyx, 1xIR4, 1xIR3
- TeraGrid Visualization cluster (ANL), Intel Xeon
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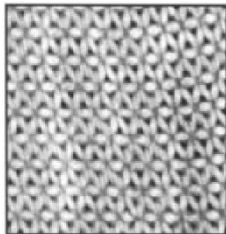
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Storage

- 20TB of data generated during project, 2TB stored at ATLAS/RAL.

Real and virtual gyroids



Gyroidic
copolymer melt

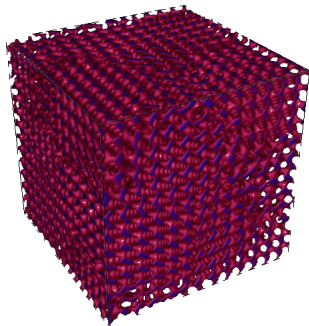


Perfect gyroid



TeraGyroid
simulation

Data still undergoing analysis



- Gyroids with defects successfully simulated
- Complete record of self-assembly and defect dynamics from the start
- Automatic detection and tracking of defects is tricky...

Conclusions

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- Modelling complex fluids is hard
- HPC makes it possible
- Computational grids allow distributed HPC resources at multiple institutions to be deployed together to attack a scientific problem.

Thanks

...and hundreds of individuals at:

TERAGRID



epcc

Argonne National Laboratory (ANL)
Boston University

BT
BT Exact
Caltech
CSC



Computing Services for Academic Research (CSAR)

CCLRC Daresbury Laboratory
Department of Trade and Industry (DTI)
Edinburgh Parallel Computing Centre

Engineering and Physical Sciences Research Council (EPSRC)
Forschungszentrum Juelich
HLRS (Stuttgart)



HPCx
CAPABILITY COMPUTING

HPCx
IBM

Imperial College London
National Center for Supercomputer Applications (NCSA)

Pittsburgh Supercomputer Center
San Diego Supercomputer Center
SCinet

NCSA

sgi



SGI
SURFnet
TeraGrid



Tufts University, Boston
UKERNA

UK Grid Support Centre
University College London
University of Edinburgh
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PITTSBURGH
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EPSRC



SURFnet