Grid Computing: Application to Science

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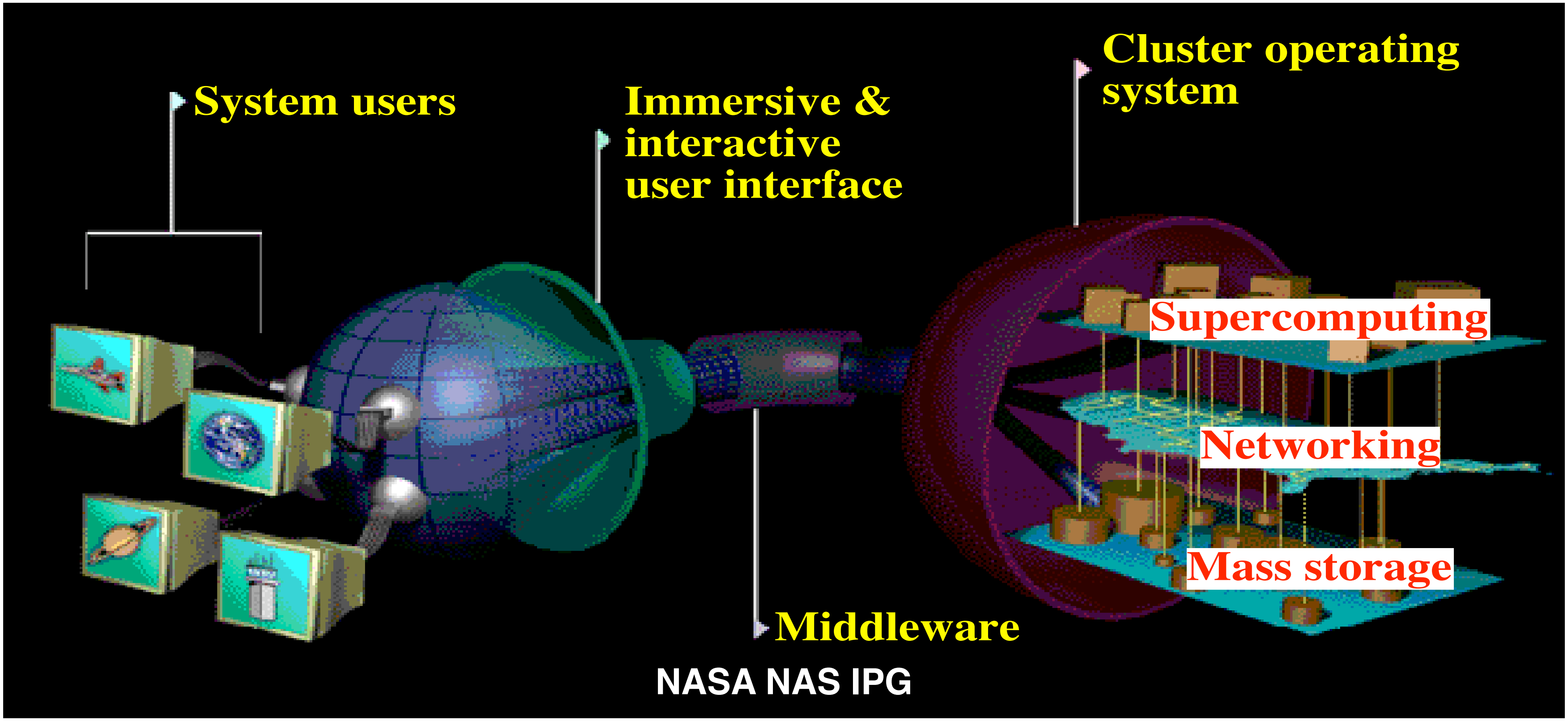
Grid = gateway to post-exascale (fault resilience, latency hiding) & cloud computing

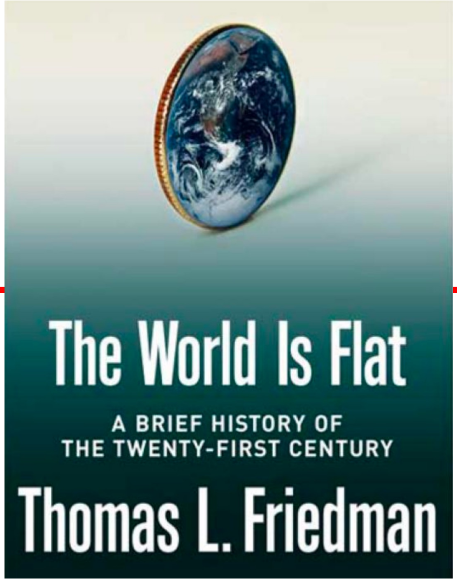
Grid Computing

- **World Wide Web:** Universal interface to digital library on the Internet
- **Information Grid:** Pervasive (from any place in the world at any time) access to everything (computing, mass storage, experimental equipment, distributed sensors, *etc*., on high-speed networks)



Scientific Grid Applications

1. **Distributed supercomputing (metacomputing):** Uses geographically distributed multiple supercomputers to tackle problems that cannot be solved on a single platform
2. **Data-intensive science:** Synthesizes new knowledge from massive data maintained in geographically distributed repositories, digital libraries & databases (Google science)
3. **Remote experimentation:** Teleoperation & teleobservation of experiments
4. **Collaborative computing:** Enable human-to-human interactions in a virtual shared space



- **Virtual community science**
  democratization of science: "Do I really need all that infrastructure to do science?"

Application-Level Grid Tools

Grid programming models

- Message passing: MPICH-G2
- Remote procedure call: Ninf-G

Grid application types

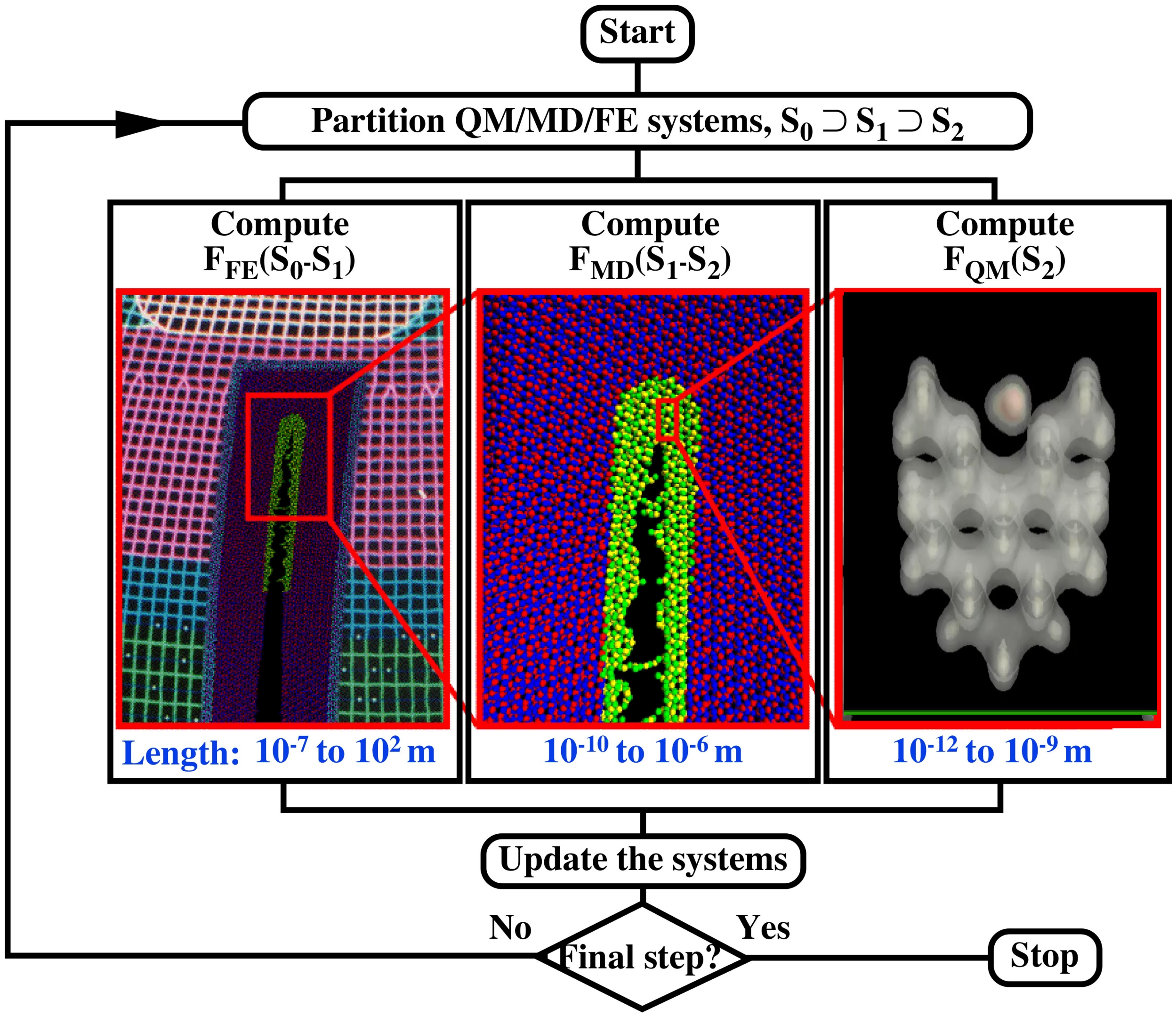
- Metacomputing
- Parameter-sweep (high throughput) applications
- Workflow applications *cf*. https://pegasus.isi.edu/
- Portals: Thin-client, graphical user interfaces to the Grid *cf*. https://nanohub.org/

Outline

1. Grid programming
   - Metacomputing—multiscale MD/quantum-mechanical (QM) simulations: Grid-enabled MPI (MPI–G2)
   - Task farm: Grid remote procedure call (Ninf–G)
   - Sustainable & adaptive Grid supercomputing
2. Grid software
   - Globus toolkit
   - Open Grid Services Architecture (OGSA)

Multiscale FE/MD/QM Simulation

- Embed high-accuracy computations only when & where needed
- Train coarse simulations by fine simulations



Multiscale simulation to seamlessly couple:

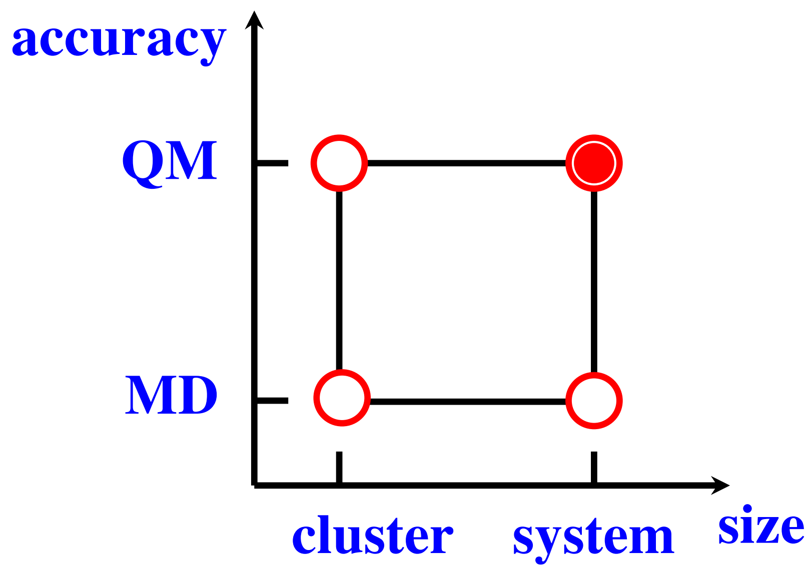
- Finite-element (FE) calculation based on continuum elasticity
- Atomistic molecular-dynamics (MD) simulation
- Quantum-mechanical (QM) calculation based on the density functional theory (DFT)

Grid-Enabled MD/QM Algorithm

Additive hybridization [Morokuma *et al*., '96]

- **Extrapolation in meta-model space (accuracy *vs*. size)**

$$E \cong E_{\mathrm{MD}}^{\mathrm{system}} + E_{\mathrm{QM}}^{\mathrm{cluster}} - E_{\mathrm{MD}}^{\mathrm{cluster}}$$

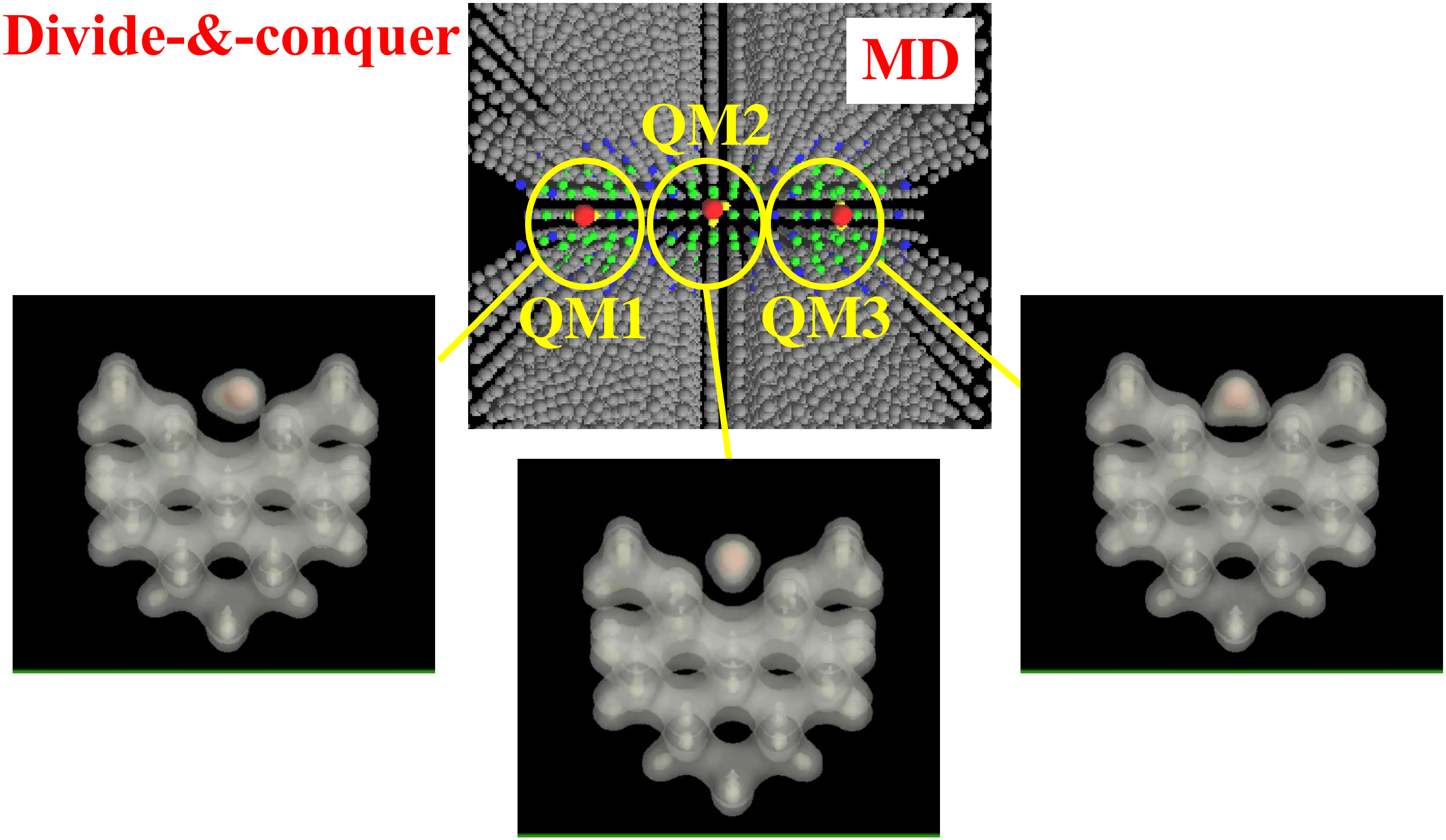


- **Modular**
  → **Reuse of existing MD & QM codes**
  → **Minimal inter-model dependence/communication**

Grid Enabling: Multiple QM Clustering

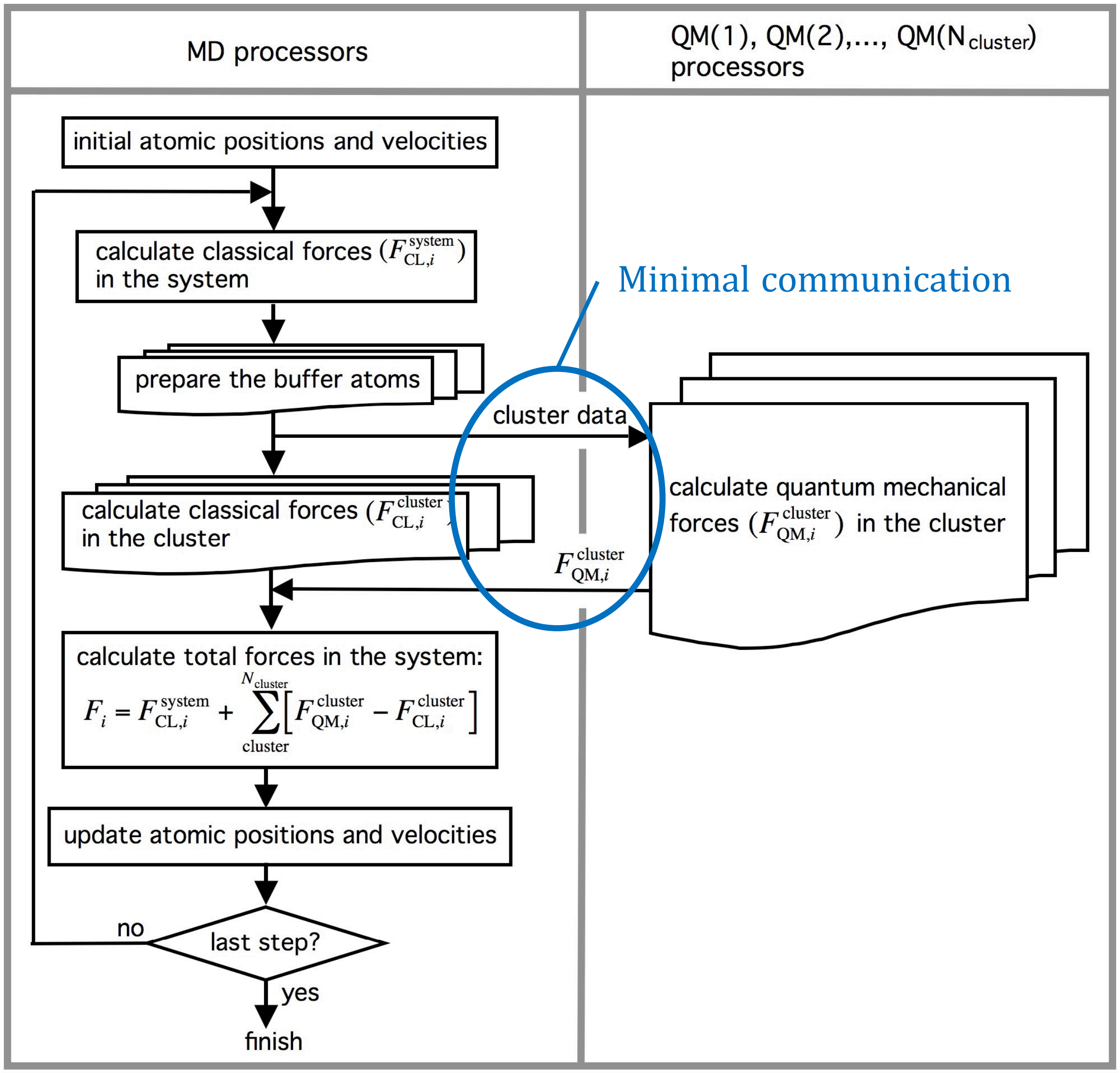
$$E = E_{\mathrm{MD}}^{\mathrm{system}} + \sum_{\mathrm{cluster}} [E_{\mathrm{QM}}^{\mathrm{cluster}}(\{\mathbf{r}_{\mathrm{QM}}\},\{\mathbf{r}_{\mathrm{HS}}\}) - E_{\mathrm{MD}}^{\mathrm{cluster}}(\{\mathbf{r}_{\mathrm{QM}}\},\{\mathbf{r}_{\mathrm{HS}}\})]$$

Divide-&-conquer



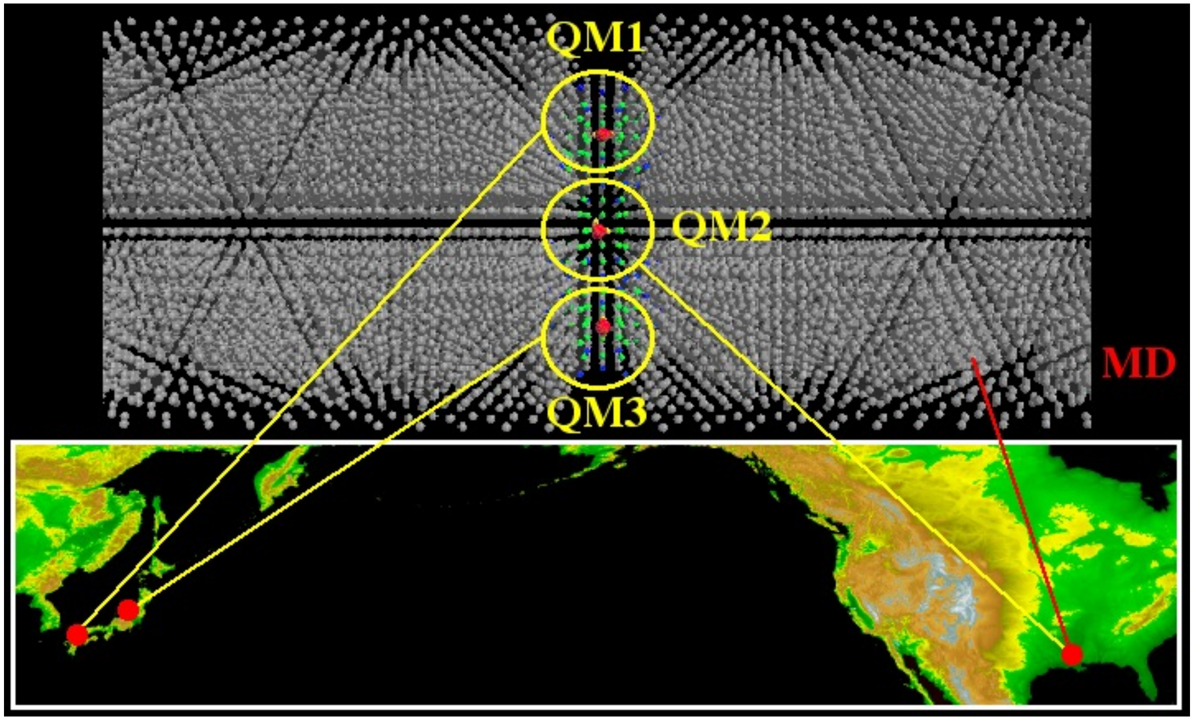
Grid Implementation

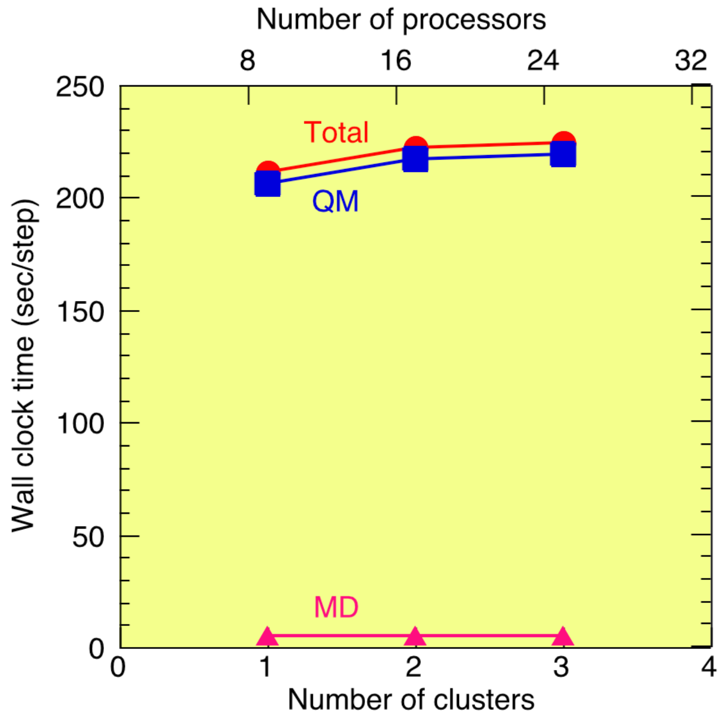
- **Task decomposition (MPI Communicator) + spatial decomposition**
- **Computation/communication overlapping to hide latency** MPI_Irecv()
- **MPICH-G2** (www3.niu.edu/mpi)**/Globus** (www.globus.org)



Global Collaborative Simulation

Hybrid MD/QM simulation on a Grid of distributed PC clusters in the US & Japan





Japan: Yamaguchi — 65 P4 2.0GHz
Hiroshima, Okayama, Niigata — 3×24 P4 1.8GHz
US: Louisiana — 17 Athlon XP 1900+

MD — 91,256 atoms
QM (DFT) — 76*n* atoms on *n* clusters

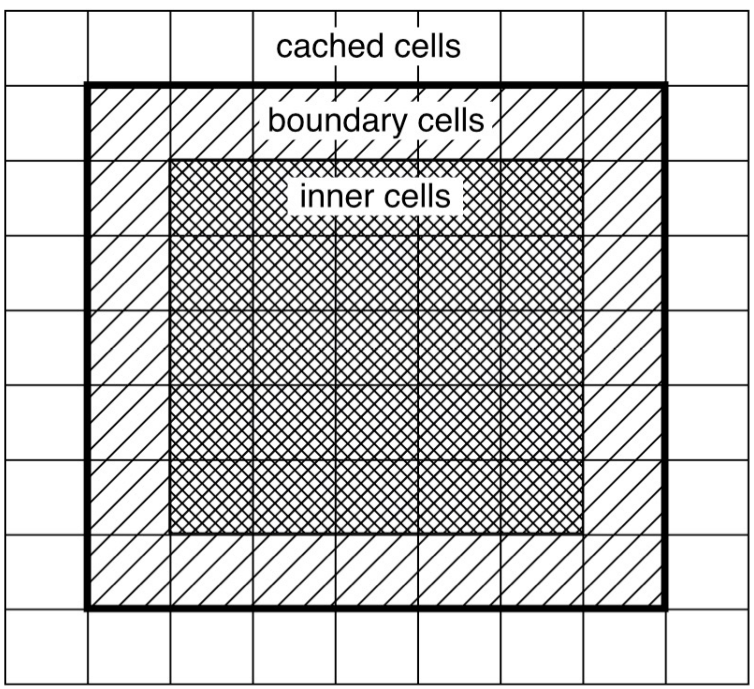
- **Scaled speedup, *P* = 1 (for MD) + 8*n* (for QM)**
- **Weak-scaling efficiency = 0.94 on 25 processors over 3 PC clusters**

H. Kikuchi *et al.*, *IEEE/ACM SC02*

Grid-Enabled MD Algorithm

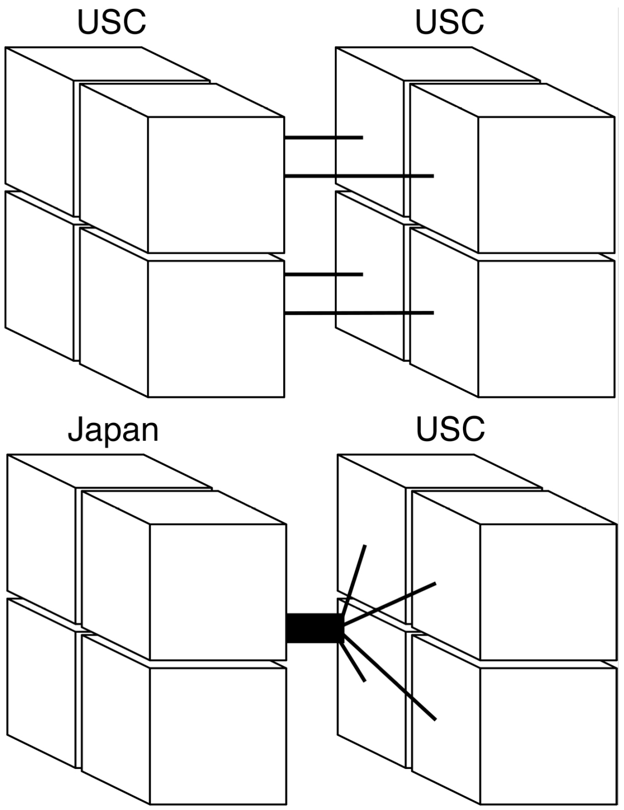
Grid MD algorithm:

1. asynchronous receive of cells to be cached MPI_Irecv()
2. send atomic coordinates in the boundary cells
3. compute forces for atoms in the inner cells
4. wait for the completion of the asynchronous receive MPI_Wait()
5. compute forces for atoms in the boundary cells



Renormalized Messages:

Latency can be reduced by composing a large cross-site message instead of sending all processor-to-processor messages



Fast TCP

BBC NEWS WORLD EDITION

Last Updated: Thursday, 5 June, 2003, 10:48 GMT 11:48 UK

E-mail this to a friend   Printable version

Promise of ultra-fast downloads

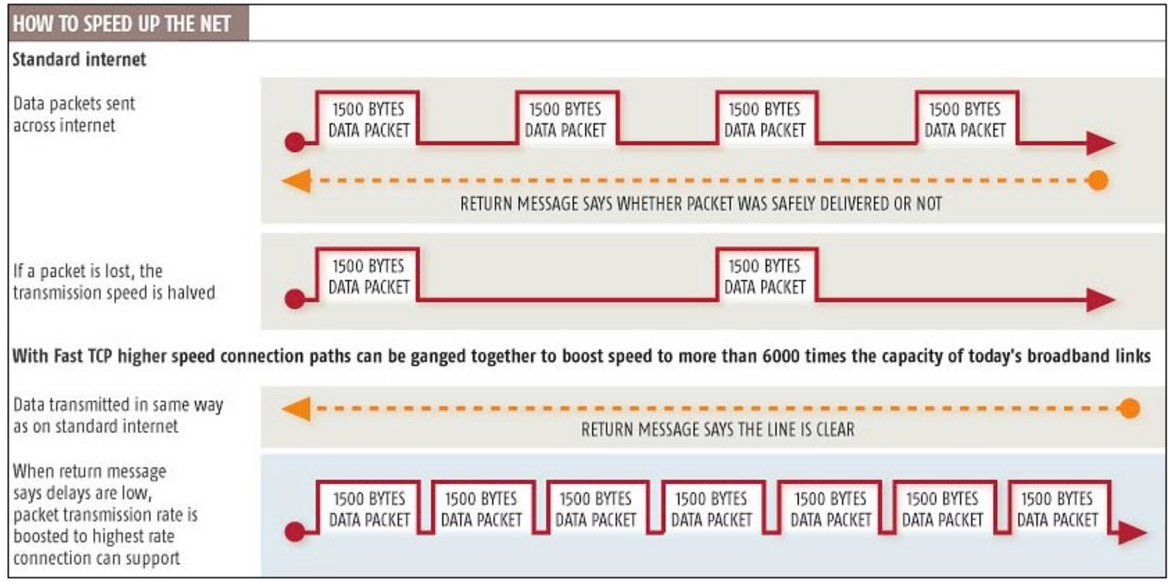
Soon you could be downloading an entire movie off the net far faster than you do now.

Fast net tech could soon take off

US researchers are working on ways to improve the way that net protocols decide how quickly data travels around the net.

Early tests of the new system show that it can triple data transmission speeds.

By linking lots of the faster systems together the researchers have produced data transfer speeds many times higher than is possible today.



Packet tracking promises ultrafast internet

10:54 05 June 03

Exclusive from New Scientist Print Edition. Subscribe and get 4 free issues.

Imagine an internet connection so fast it will let you download a whole movie in just five seconds, or access TV-quality video servers in real time. That is the promise from a team at the California Institute of Technology in Pasadena, who have developed a system called Fast TCP.

Fast TCP: Achieved 8.6 Gb/s between Sunnyvale, CA & CERN, Switzerland

Steven Low (Caltech)

http://netlab.caltech.edu/FAST

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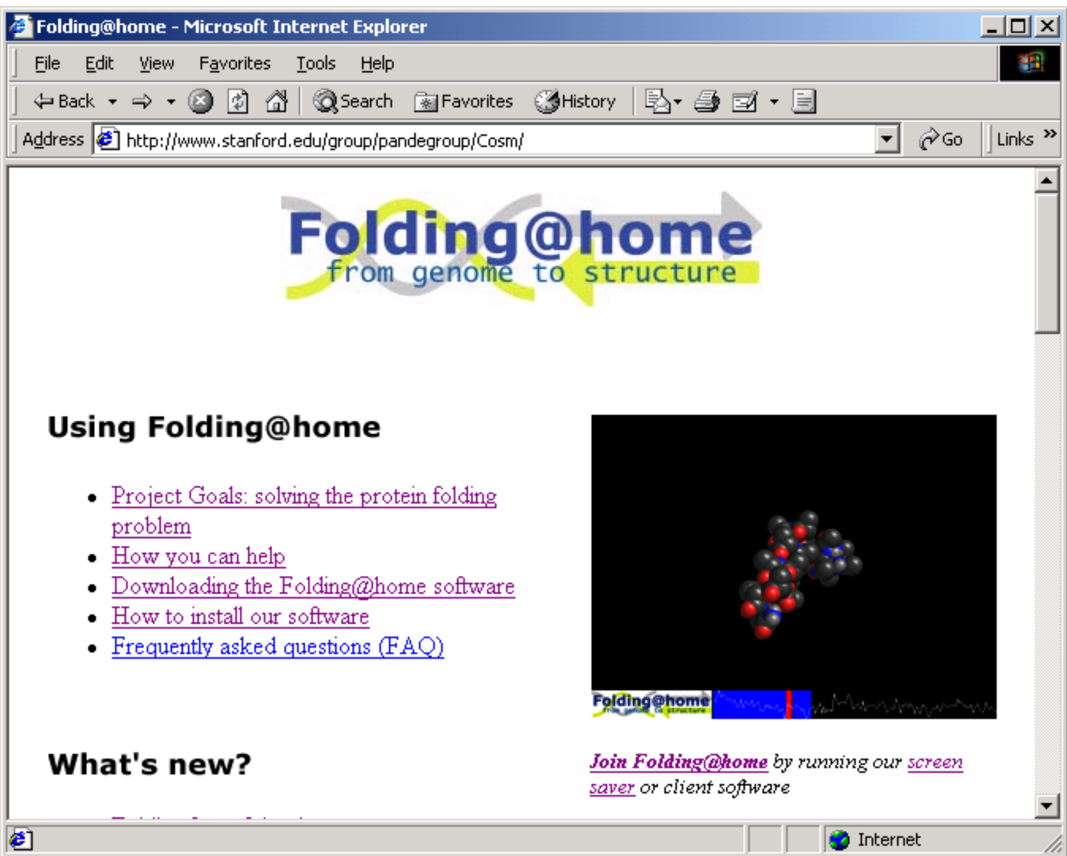
   > Globus toolkit
   > Open Grid Services Architecture (OGSA)

Task Farm Applications

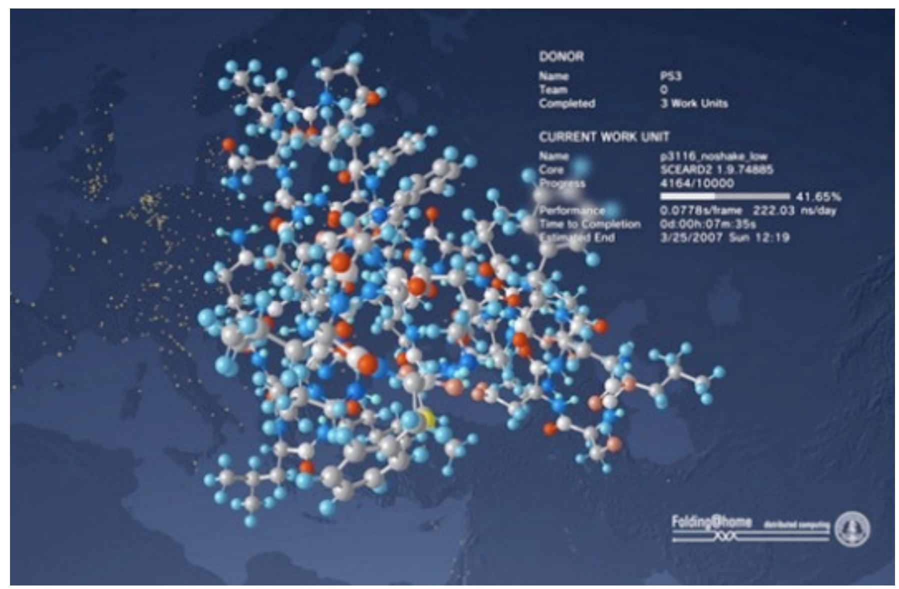
cf. Protein folding in [2024 Nobel Chemistry Prize]

Number CPUs	Number Active CPUs	Number Users	Number Teams	Last Update
423995	90438	210257	25971	2003-05-05 20:04:04

OS type	Active	Total
Windows	86473	369859
Mac OS X	2653	24129
Linux	1294	29931
Other	0	13
Total	90420	423932



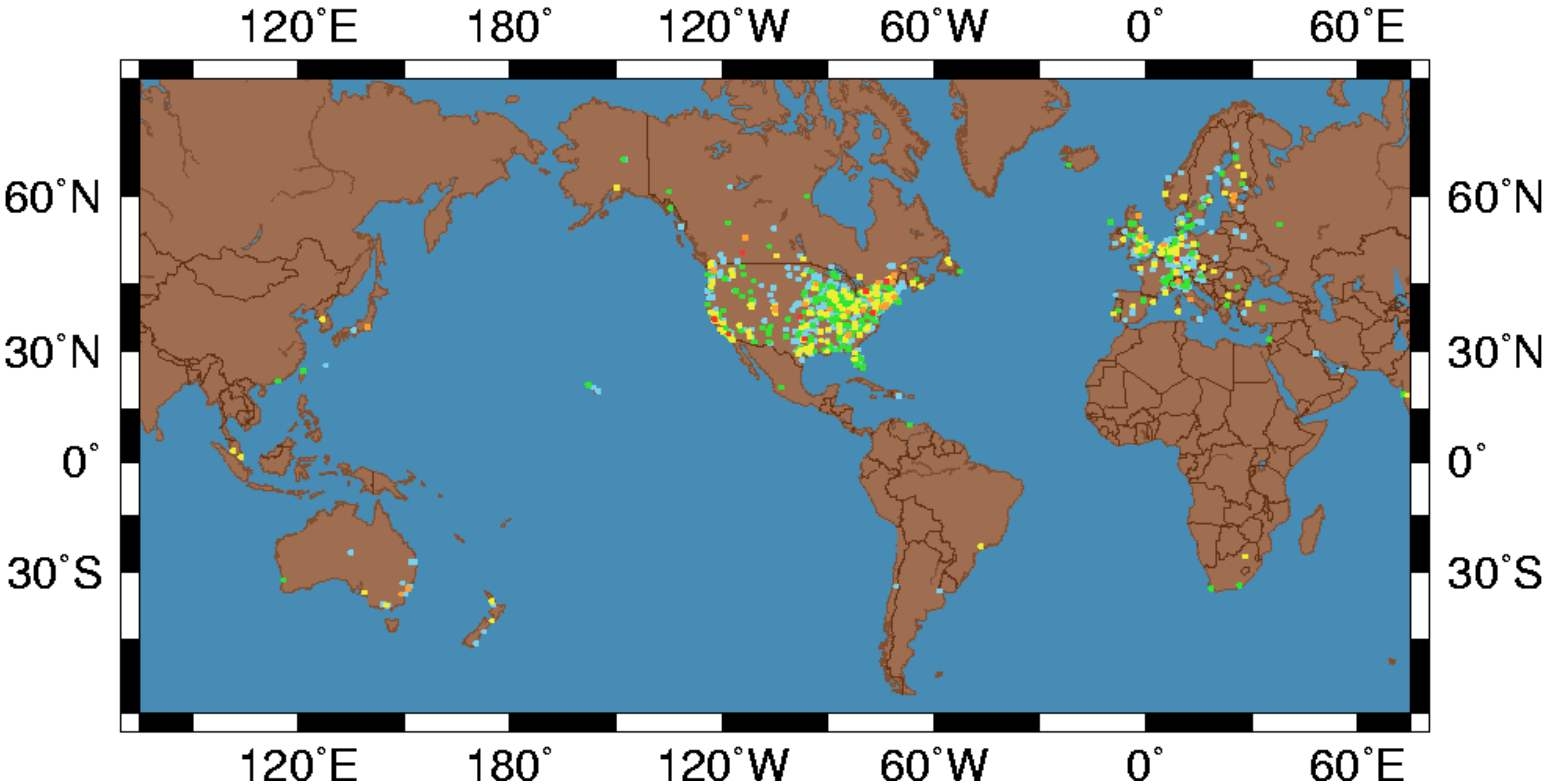
Screen saver
(*cf.* OpenGL idle event handler)



https://foldingathome.org/home

World Wide Distributed Computing

Folding@home



https://foldingathome.org/home

Enabling Science by Online Game

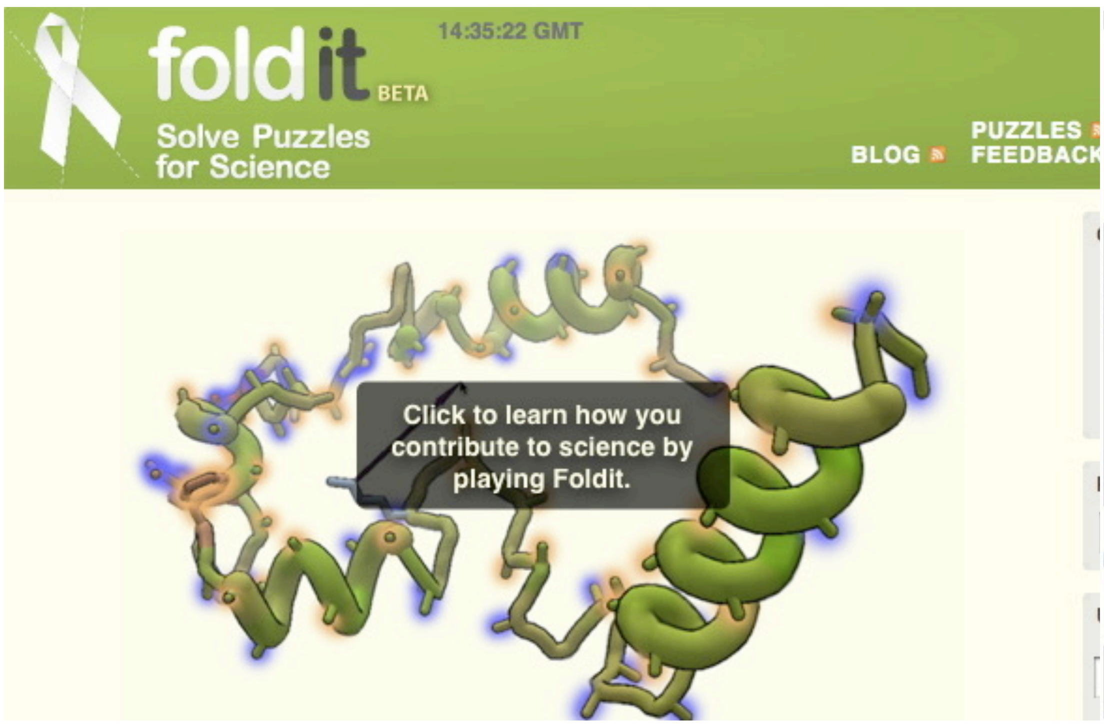
nature Vol 466|5 August 2010|doi:10.1038/nature09304

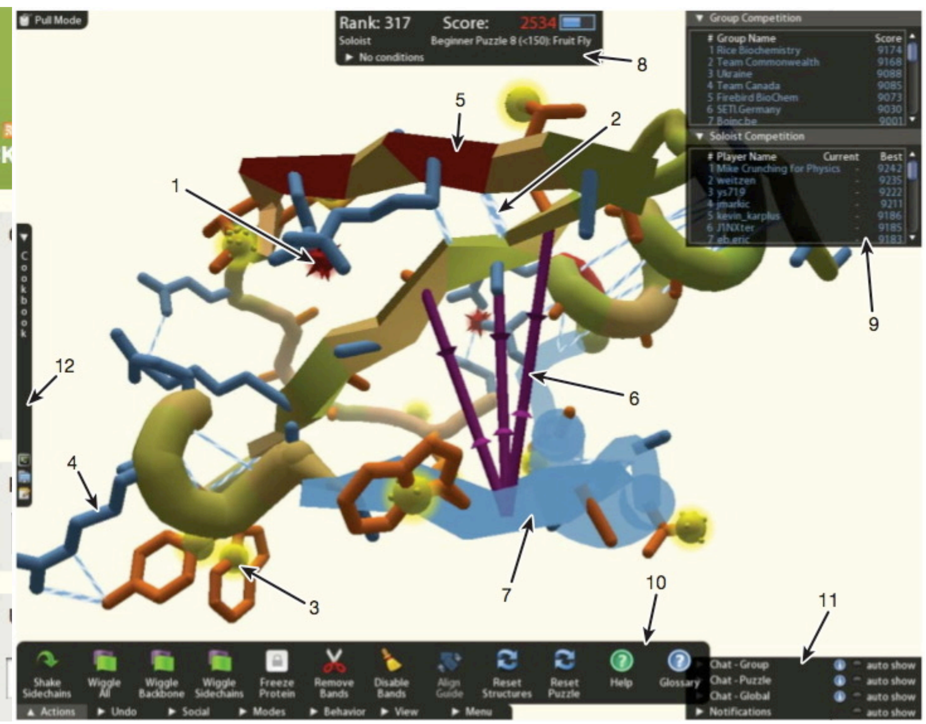
LETTERS

From passive to active users

Predicting protein structures with a multiplayer online game

Seth Cooper[1], Firas Khatib[2], Adrien Treuille[1,3], Janos Barbero[1], Jeehyung Lee[3], Michael Beenen[1], Andrew Leaver-Fay[2]†, David Baker[2,4], Zoran Popović[1] & Foldit players

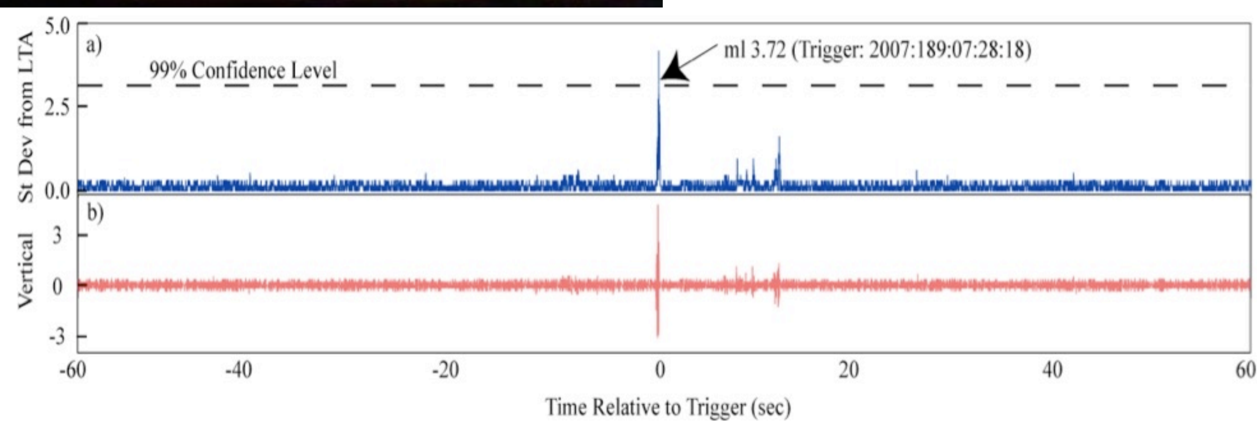




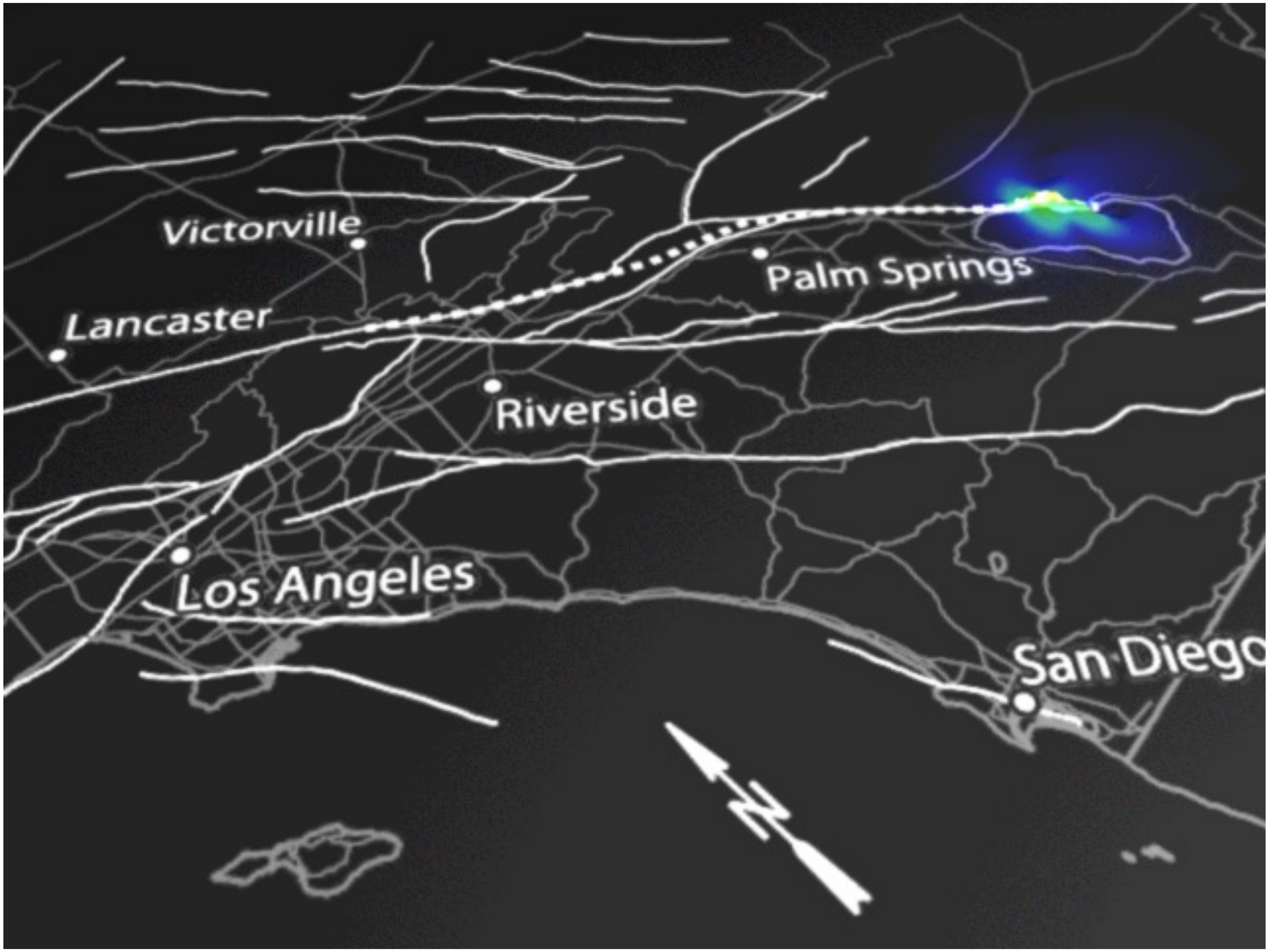
Quake-Catcher Network

- Network of accelerometer-equipped laptops/desktops for early earthquake warning & research
- Clustering accelerometer time series data to detect earthquakes

https://quakecatcher.net



Virtual Earthquake: Atomic to Tectonic



Southern California Earthquake Center (SCEC)

Thomas Jordan http://www.scec.org

Harvard Clean Energy Project

http://cleanenergy.molecularspace.org

world community grid.
technology solving problems

What's New

World Community Grid: now available on Android!

Your smartphone or tablet can now help search for the next HIV treatment. Join today or add your Android device to your existing account.

Learn more

Who We Are

World Community Grid brings together people from across the globe to benefit humanity by creating the world's largest non-profit computing grid. We do this by pooling surplus processing power from volunteers' devices. We believe that innovation combined with visionary scientific research and large-scale volunteerism can help make the planet smarter. Our success depends on like-minded individuals - like you.

How You Can Help

Download and install secure, free software that captures the spare processing power of your computer, smartphone or tablet, and harnesses it for scientific research.

Join Today!

What's New

The Clean Energy Project data published!

Harvard researchers published their database with the electronic properties of 2.3 million organic compounds. What might this mean for the future of solar cells?

http://www.worldcommunitygrid.org

Scrödinger—Cycle Computing—USC

March 28, 2014 http://www.hpcwire.com

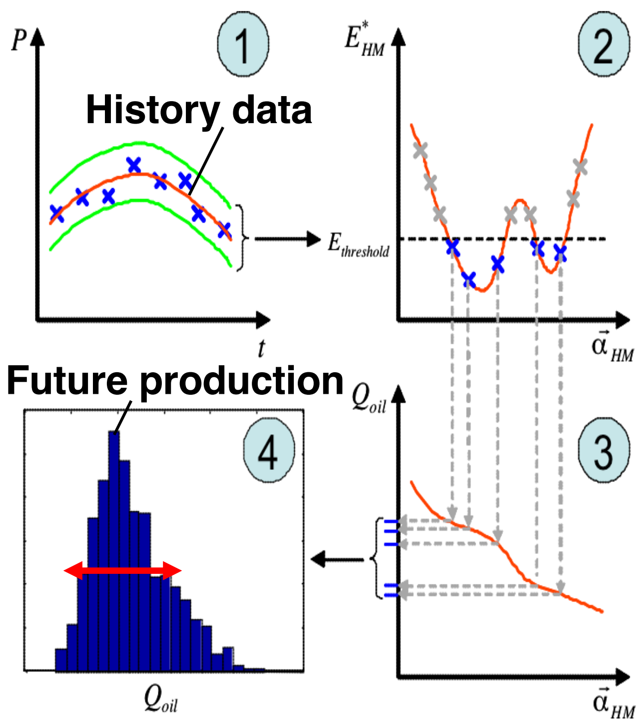
Schrödinger Partners with Cycle Computing to Accelerate Materials Simulation

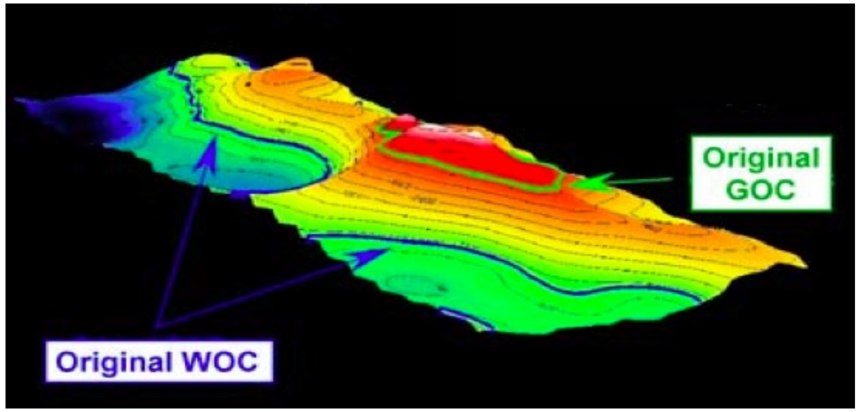
NEW YORK, N.Y., March 28 — Schrödinger, LLC and Cycle Computing, LLC announced today a partnership that will allow customers to run Schrödinger's Materials Science Suite on the Cloud and elastic resources worldwide using Cycle Computing's CycleCloudä orchestration software. Cloud Computing provides users timely access to scalable computational resources as needed, without prohibitive upfront capital investment in infrastructure. Cycle Computing and Schrödinger have worked together on enabling many customer production workloads in the cloud, including the world's largest and fastest cloud computing run of more than 156,000 cores called the MegaRun in late 2013.

During the record-breaking MegaRun, Professor Mark Thompson at the University of Southern California (USC) completed the largest cloud-computing run in the world, using Schrödinger's software running on the CycleCloud platform. Professor Thompson calculated the optoelectronic properties for 205,000 materials with potential application in organic photovoltaic devices. The run used a maximum of 156,000+ CPU-cores completing 264 CPU-years of simulation in less than 18 hours.

Parallel History Matching

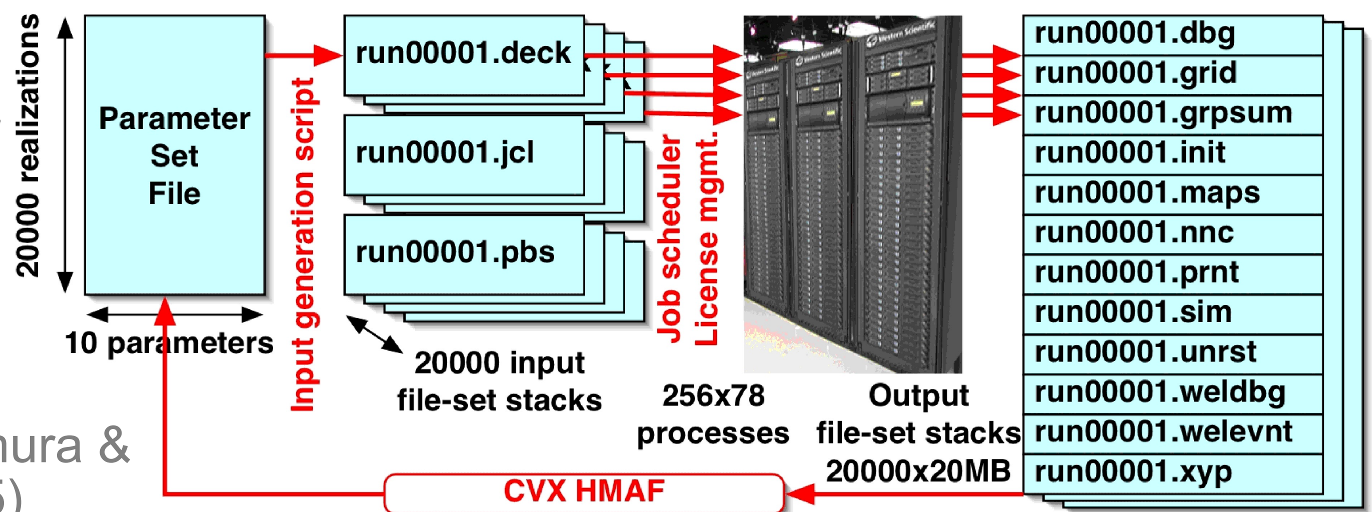
- **Inverse problem: Calibration of reservoir simulation models to the observed production data**





- Real field—offshore Africa
- 32 wells
- 30 years production history
- 30 years production forecast

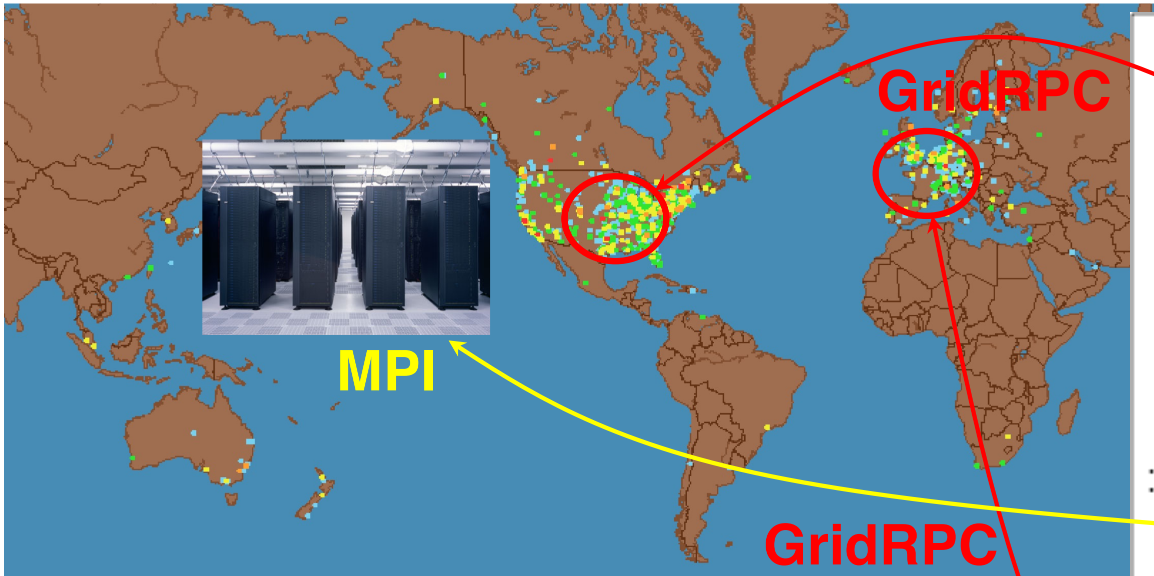
- **CVX History Match & Associated Forecast (HMAF) framework: History matching & the assessment of uncertainties associated with flow prediction**

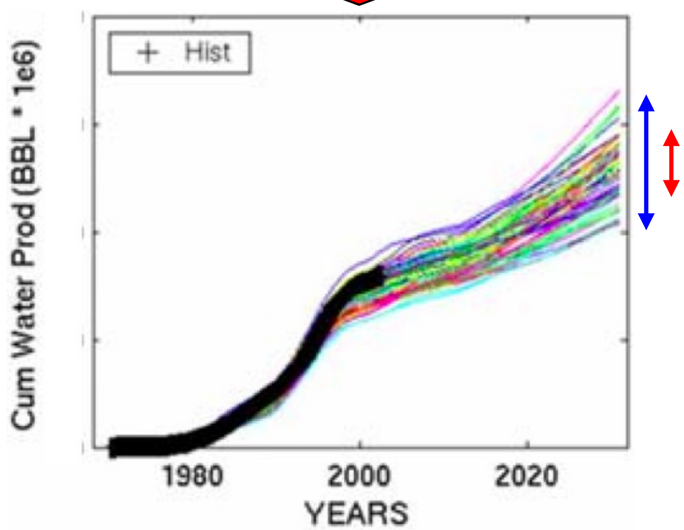


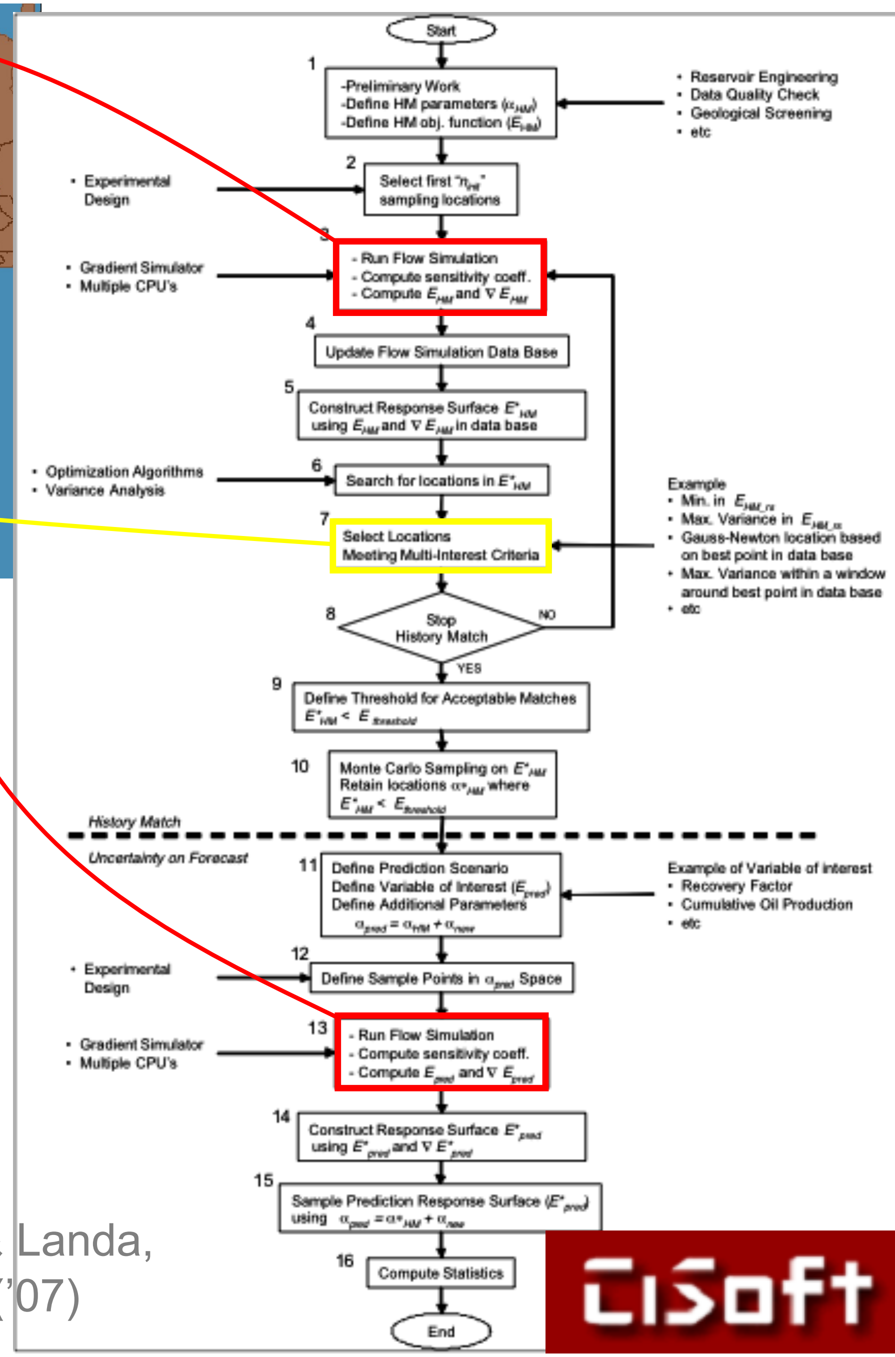
HMAF:
Landa & Guyaguler,
SPE 84465 ('03)

Parallel HMAF:
Landa, Kalia, Nakano, Nomura & Vashishta, *IPTC* 10751 ('05)

Overnight History Matching on a Grid







Nomura, Kalia, Nakano, Vashishta & Landa, *Journal of Supercomputing* **41**, 109 ('07)

CiSoft

Grid Remote Procedure Call (RPC)

- **Simple RPC API (application program interface)**
- **Existing libraries & applications into Grid applications**
- **IDL (interface definition language) embodying call information, with minimal client-side management**

```
double A[n][n],B[n][n],C[n][n];      /* Data Declaration */
dmmul(n,A,B,C);                       /* Call local function */

grpc_function_handle_default(&hdl, "dmmul");
grpc_call(hdl,n,A,B,C);   /* Call server side routine */
```

- **Ninf–G Grid RPC system**
  http://ninf.apgrid.org

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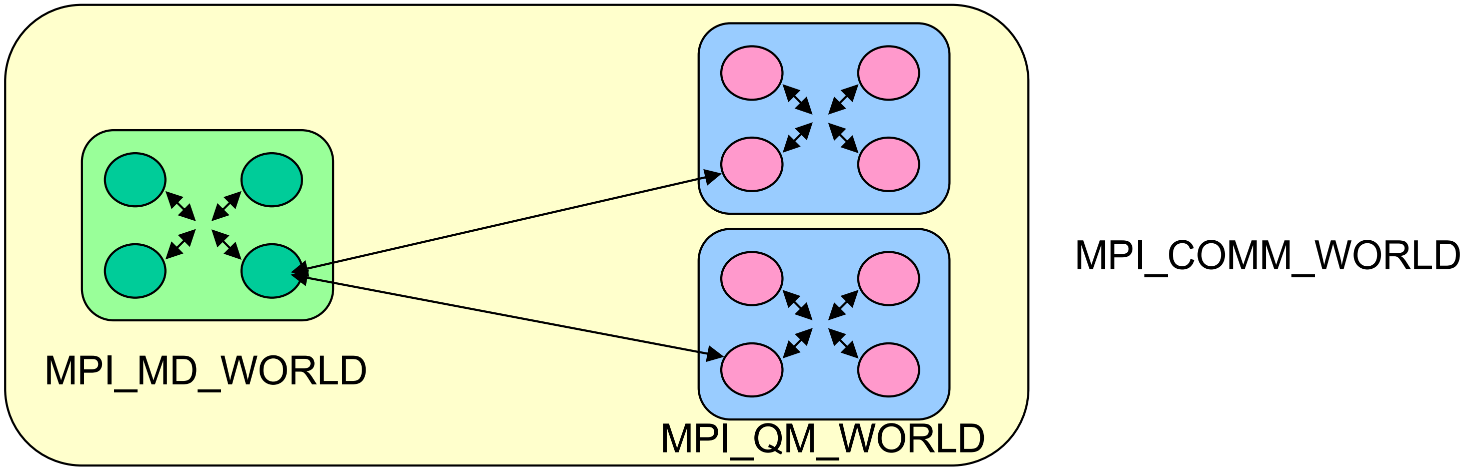
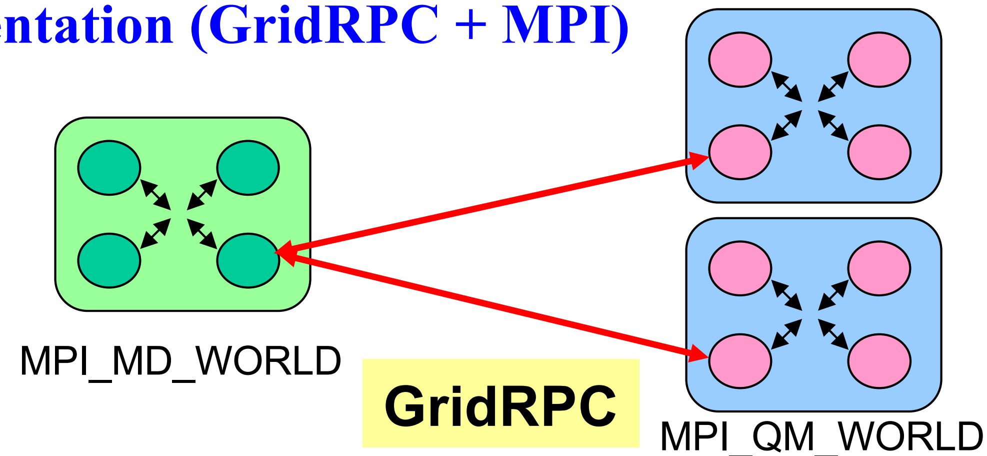
Combined GridRPC+MPI MD/QM

- **Original implementation (MPICH-G2)**

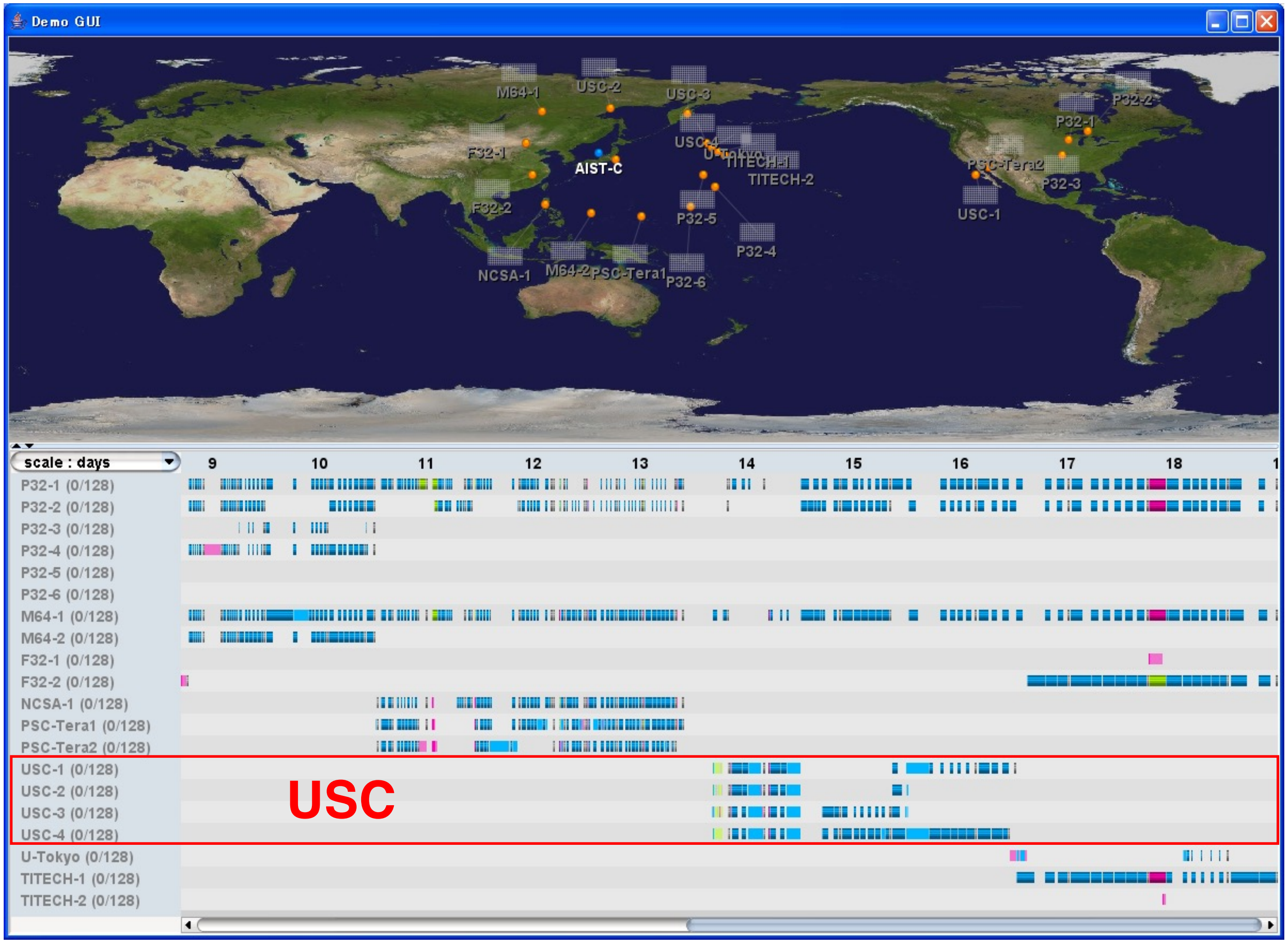


- **Hybrid implementation (GridRPC + MPI)**



- **Flexibility: Dynamically add/subtract, allocate, & migrate resources**
- **Fault tolerance: Automatically detect & recover from explicit (OS down or disconnected networks) & implicit (job stuck in a queue) faults**
- **Scalability: Manage 1000's of computing resources efficiently**

Global Grid QM/MD



H. Takemiya,
Y. Tanaka,
S. Sekiguchi
(AIST)

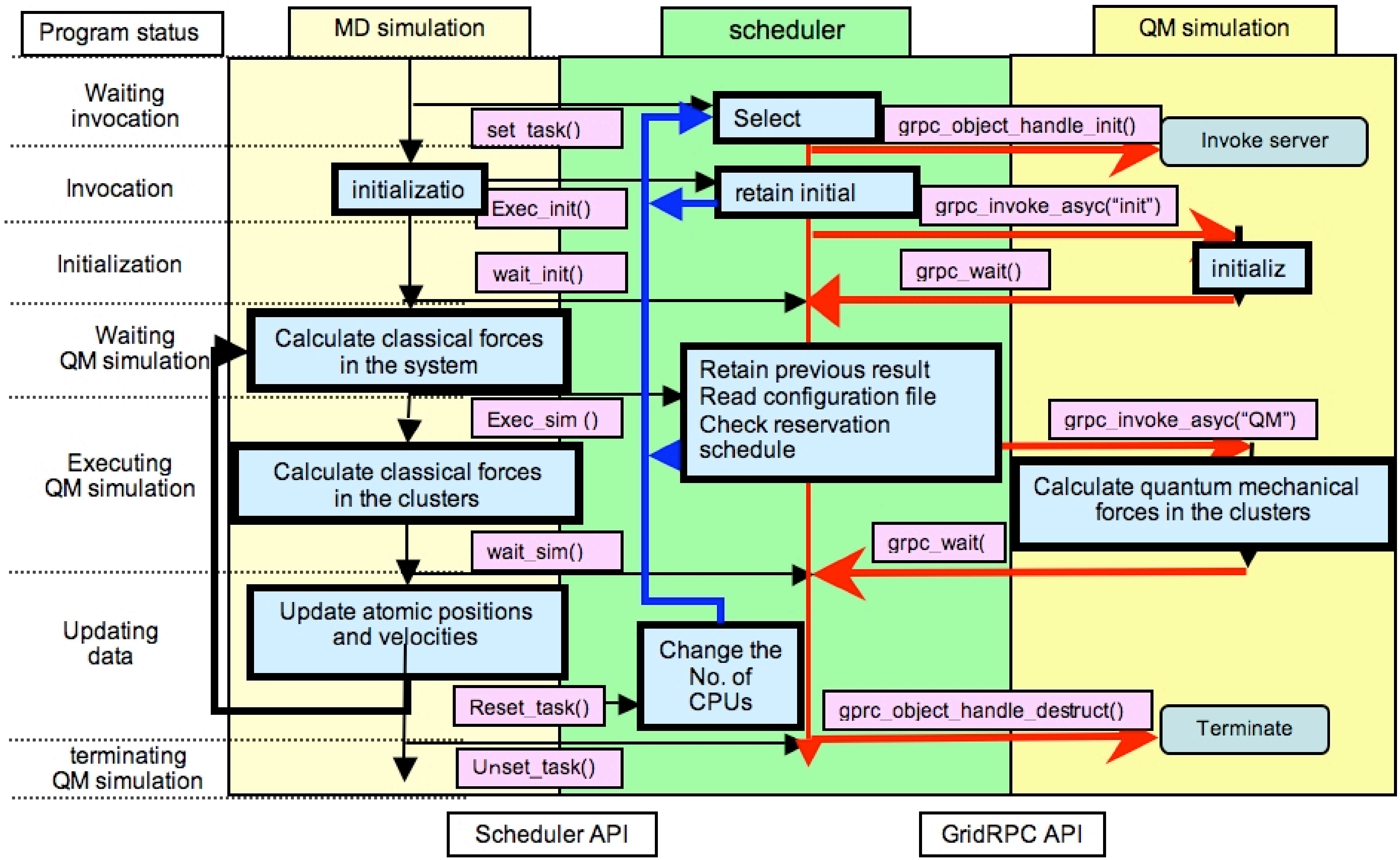
S. Ogata
(NIT)

R.K. Kalia,
A. Nakano, P. Vashishta
(USC)

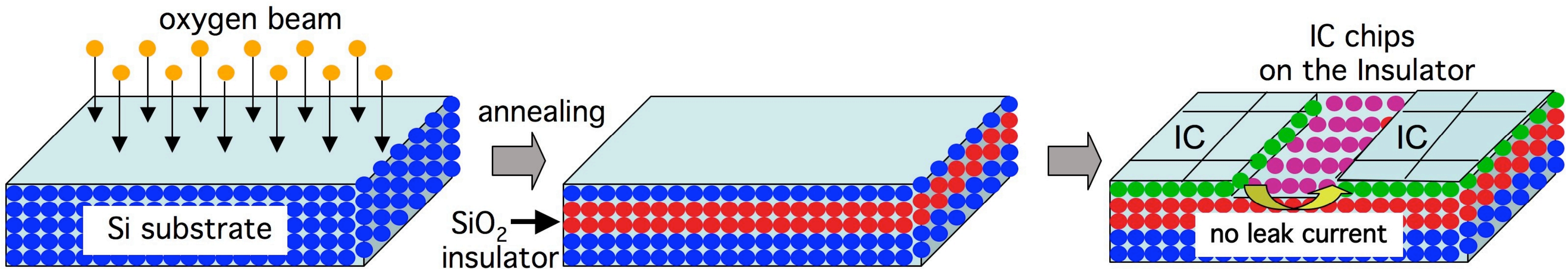
- **Hybrid GridRPC**(ninf.apgrid.org)**+MPI**(www.mcs.anl.gov/mpi) **Grid computing**
- **153,600 cpu-hrs metacomputing at 6 sites in the US (USC, PSC—Pittsburgh, NCSA—Illinois) & Japan (AIST, U Tokyo, TITech)**

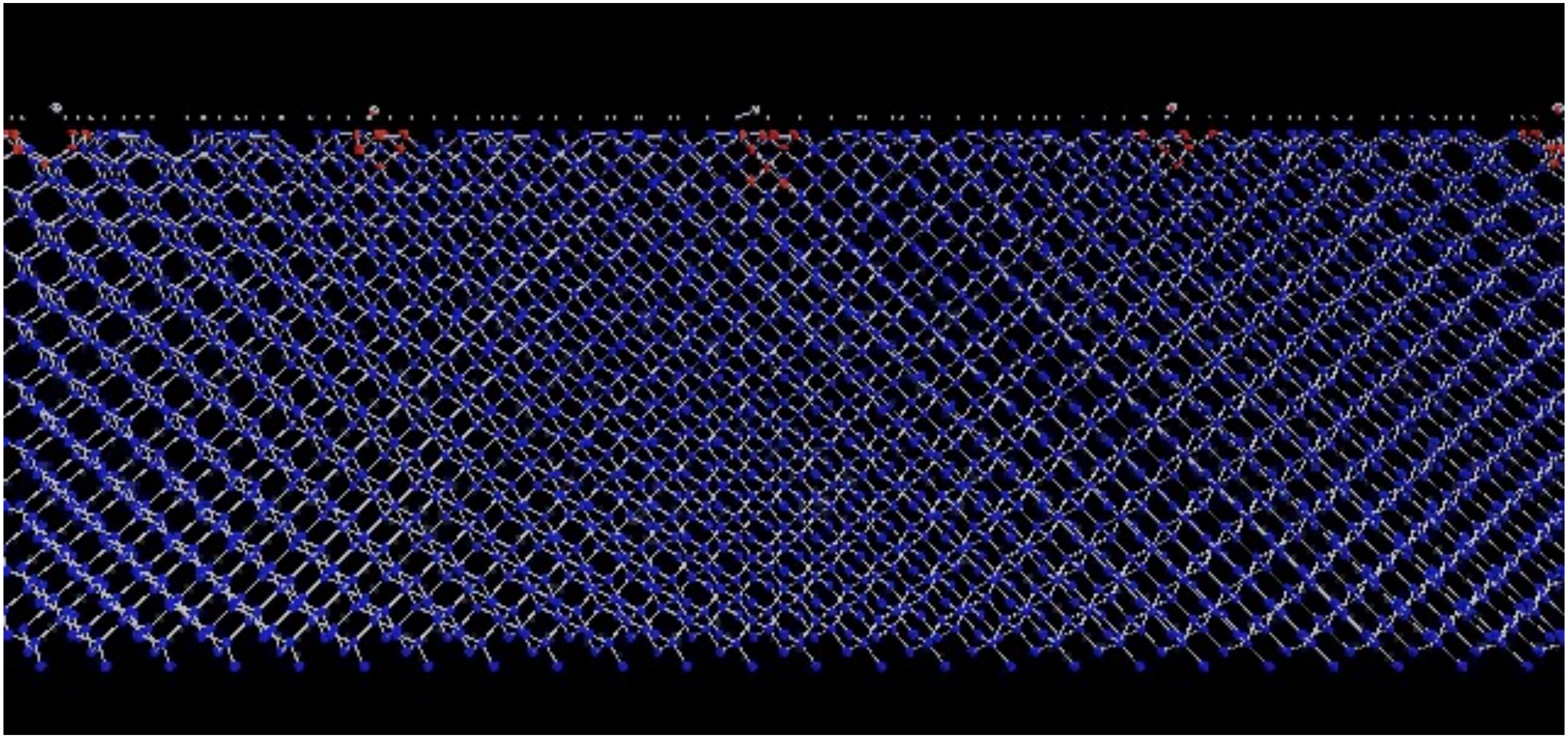
H. Takemiya *et al.*, *Proc. IEEE/ACM SC06*; Y. Song *et al.*, *Int'l J. Comput. Sci.* ('09); *CCGrid09*

Flow Chart of Grid MD/QM



SIMOX (Separation by Implantation by Oxygen)

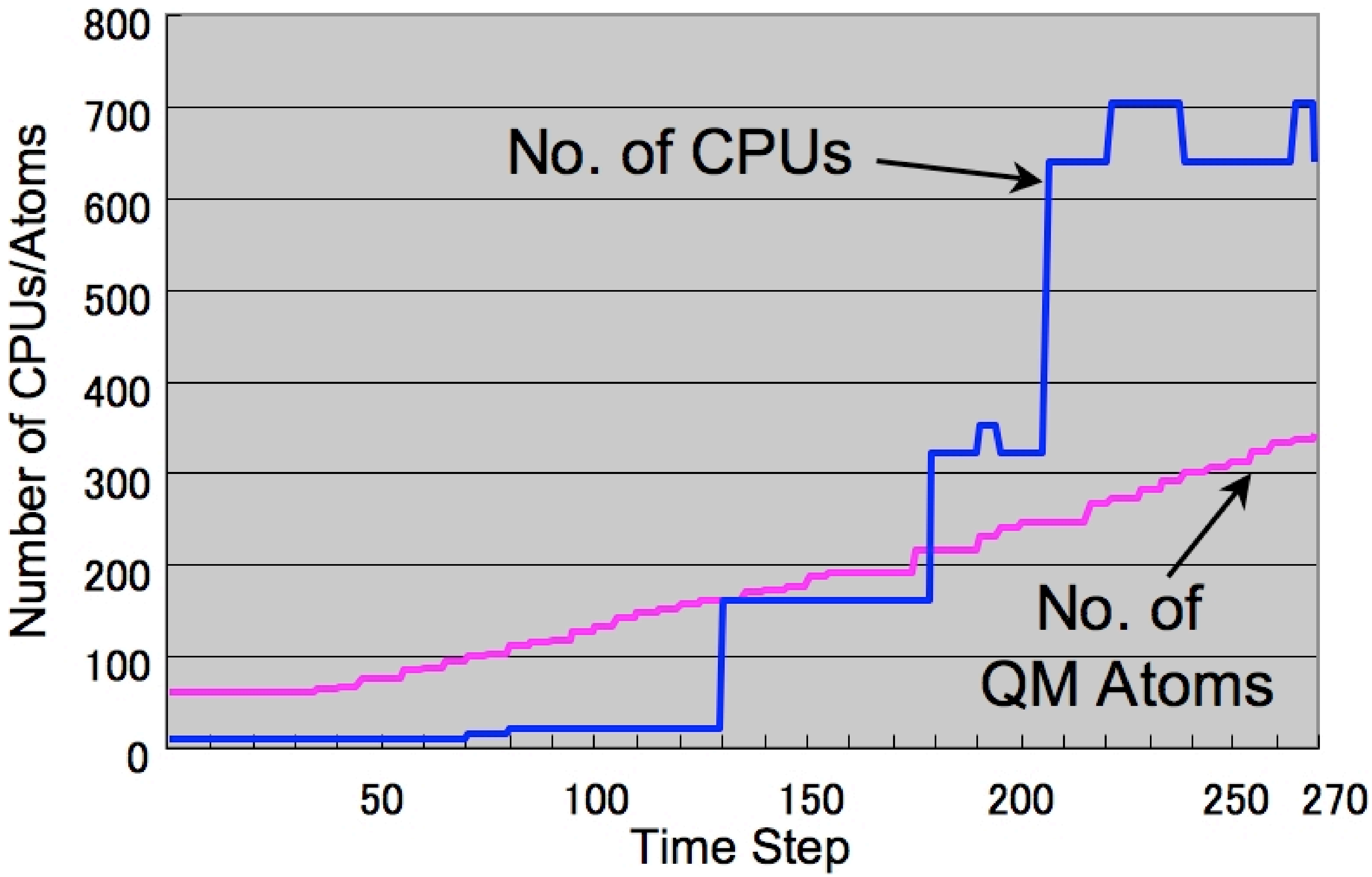




Red: quantum mechanically treated atoms ~ $O(N^3)$

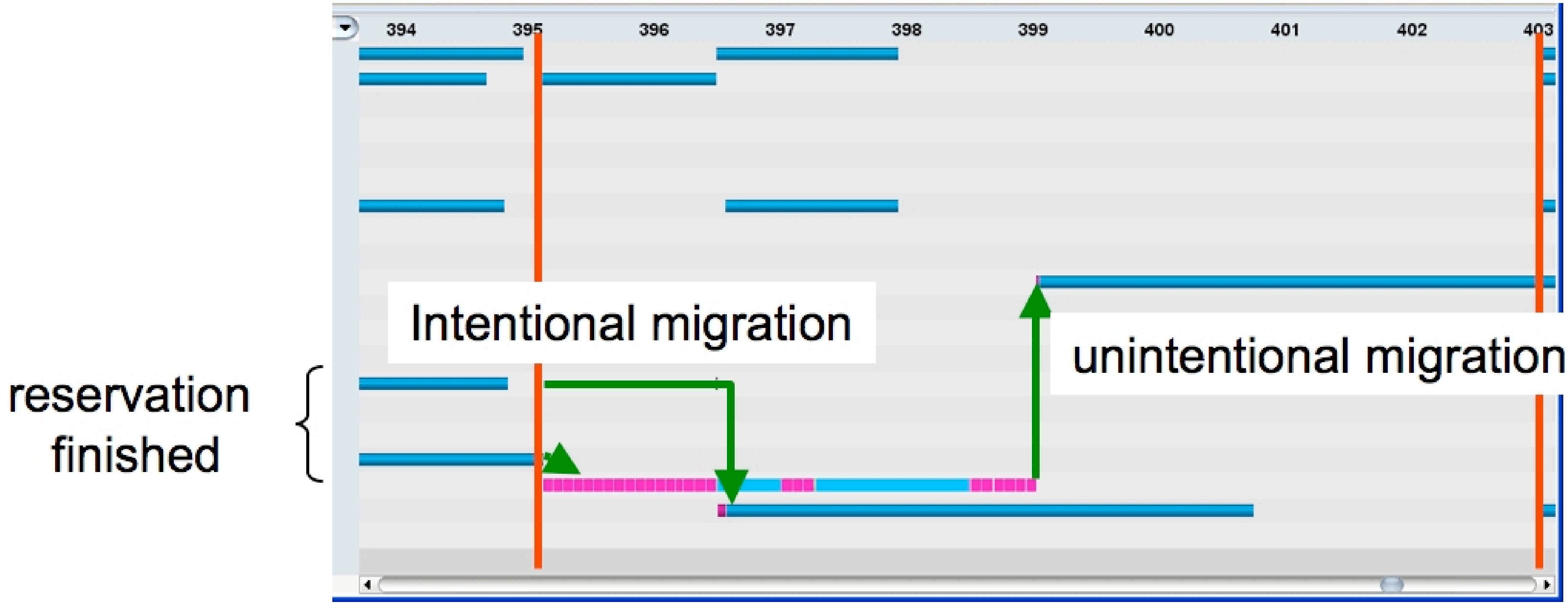
Flexibility: Adaptive MD/QM

- **Flexibility:** Automated increase of the number of QM atoms on demand to maintain accuracy & associated dynamic re-allocation of CPUs



Fault Tolerance

- **Automated migration in response to unexpected faults**



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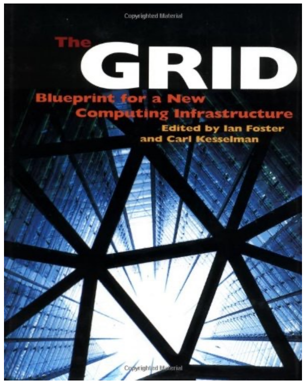
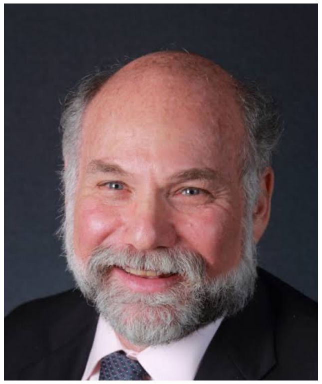
2. Grid software (1998-2018)*
   > Globus toolkit
   > Open Grid Services Architecture (OGSA)

Ian Foster (ANL)





Carl Kesselman (USC)

*USC-CARC uses Globus for file transfer

https://www.carc.usc.edu/user-guides/research-data-management/transferring-data/transferring-data-globus

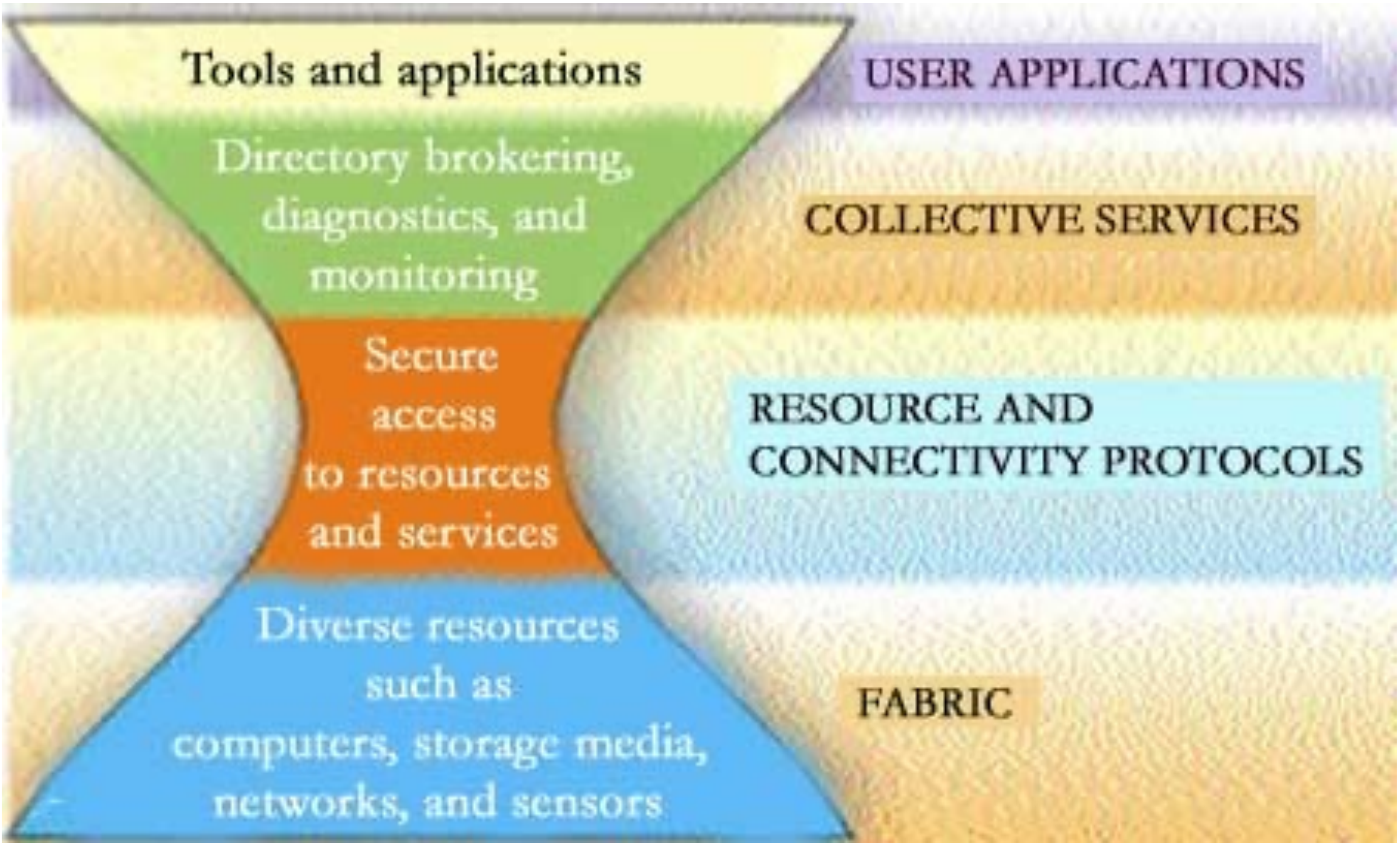
Grid System

Goal: **Coordinated resource sharing & problem solving in dynamic, multi-institutional virtual organizations.**

1. **Coordinate distributed resources.**
2. **Use standard, open, general-purpose protocols & interfaces.**
3. **Deliver nontrivial qualities of services (QoS).**

Grid Architecture

Layered architecture



- **Hourglass model: A small set of core protocols (*e.g*., TCP/IP) + various: (1) high-level behaviors & (2) underlying technologies.**

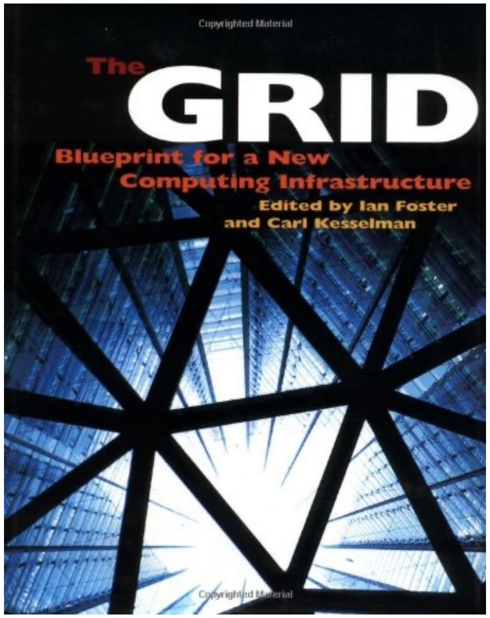
Layered Grid Architecture

- **Fabric:** Introspection & management of local resources.
  - > **Computational resources:** Start programs & monitor/control the execution of the resulting processes.
  - > **Storage:** Put & get files (*e.g.*, disk space allocation).
  - > **Network:** Control network transfers (*e.g.*, prioritization).
- **Connectivity:** Define communication & authentication protocols.
- **Resource:** Define protocols for negotiation, initiation, monitoring, control, accounting & payment of sharing operations on individual resources.
- **Collective:** Capture interactions across collection of resources, *e.g.*, directory services, co-allocation & data replication.

Globus Toolkit (1998-2018)

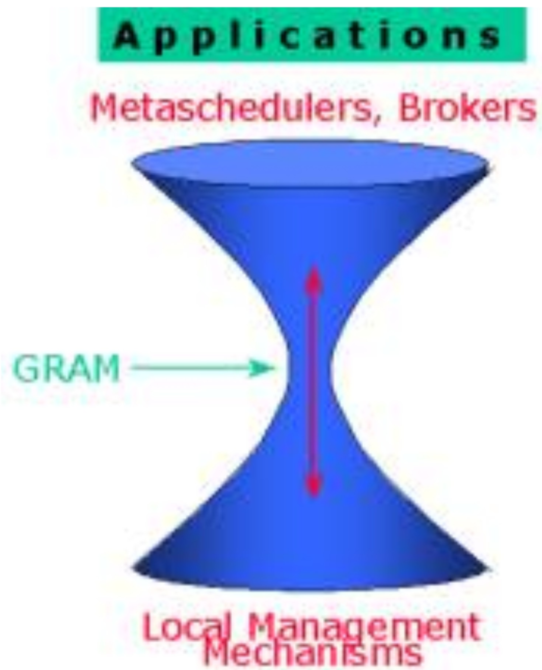
- **Globus Toolkit version 2 (GT2): Open source, de facto standard of Grid computing middleware to construct interoperable Grid applications ('97)**
  - **Define & implement protocols, application program interfaces (APIs) & services**
  - **Provide solutions to authentication, resource discovery & resource access**
- **Globus Toolkit version 3 (GT3): OGSA-compliant standard ('02)**
- **Globus Toolkit version 6 (GT6) at** http://www.globus.org

globus



GT2: Globus Toolkit 2

- **Fabric**
  > General purpose architecture for reservation & allocation (GARA)
- **Connectivity**
  > Grid security infrastructure (GSI)
- **Resource**
  > Grid resource allocation & management (GRAM) protocol



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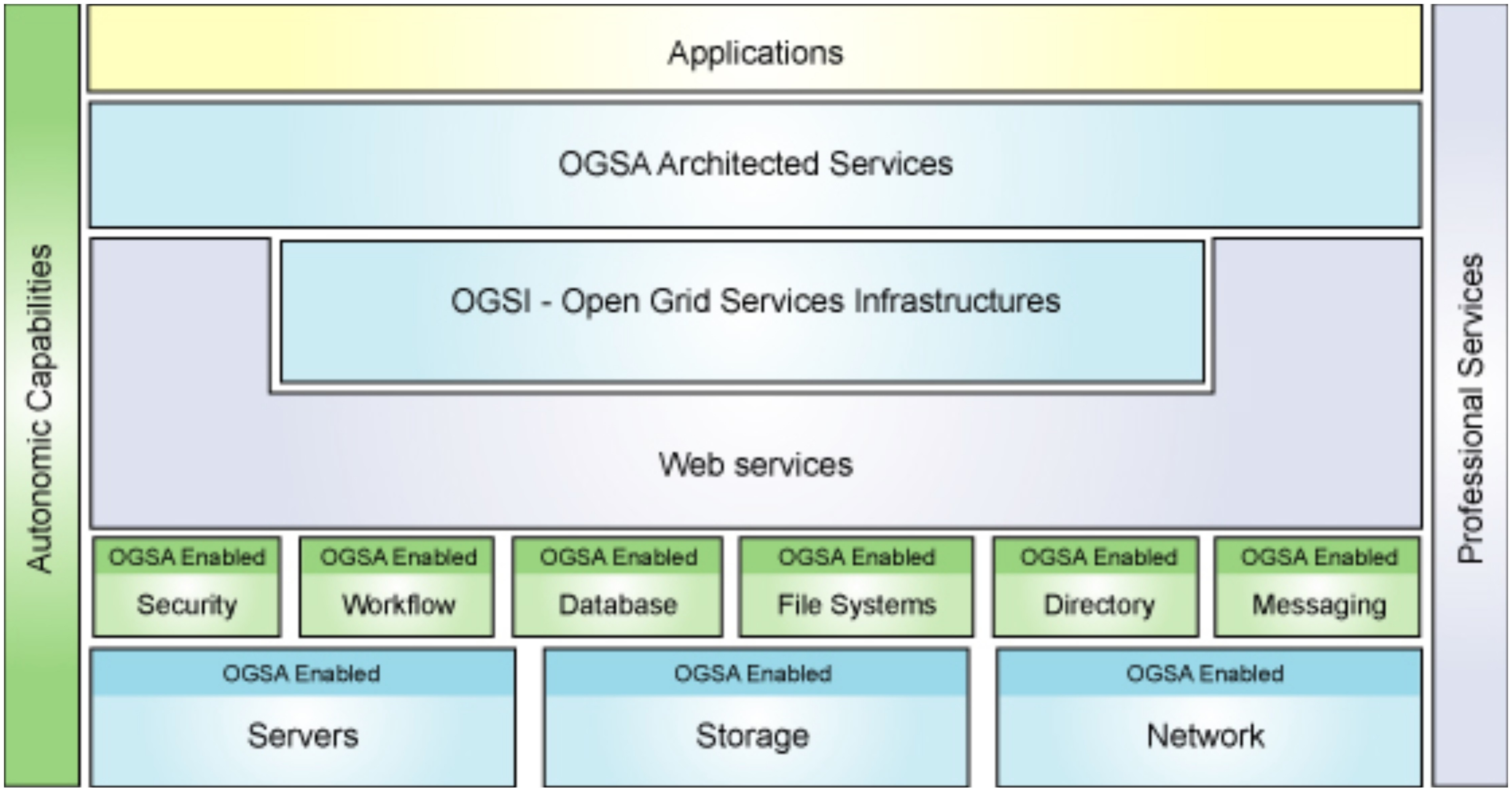
Open Grid Services Architecture (OGSA)

- **OGSA = Definition of a service-oriented infrastructure**
- **Service: A network-enabled entity with a well-defined interface that provides some capability**

1. **Align Grid computing with industrial initiatives in service-oriented architecture & Web services**
2. **Provide a framework within which to define interoperable & portable services**
3. **Define a core set of standard interfaces & behaviors**
4. **Implemented in the OGSA-based Globus Toolkit 3 (currently GT 6.0):**
   http://www.globus.org

Open Grid Services Architecture (OGSA)

1. **Web services description language (WSDL): An interface definition language describing services (or software components) independent of platforms.**
2. **Open grid services infrastructure (OGSI): A set of WSDL interfaces & associated conventions, extensions & refinements to Web services standards to support basic Grid.**



OGSI Functionalities

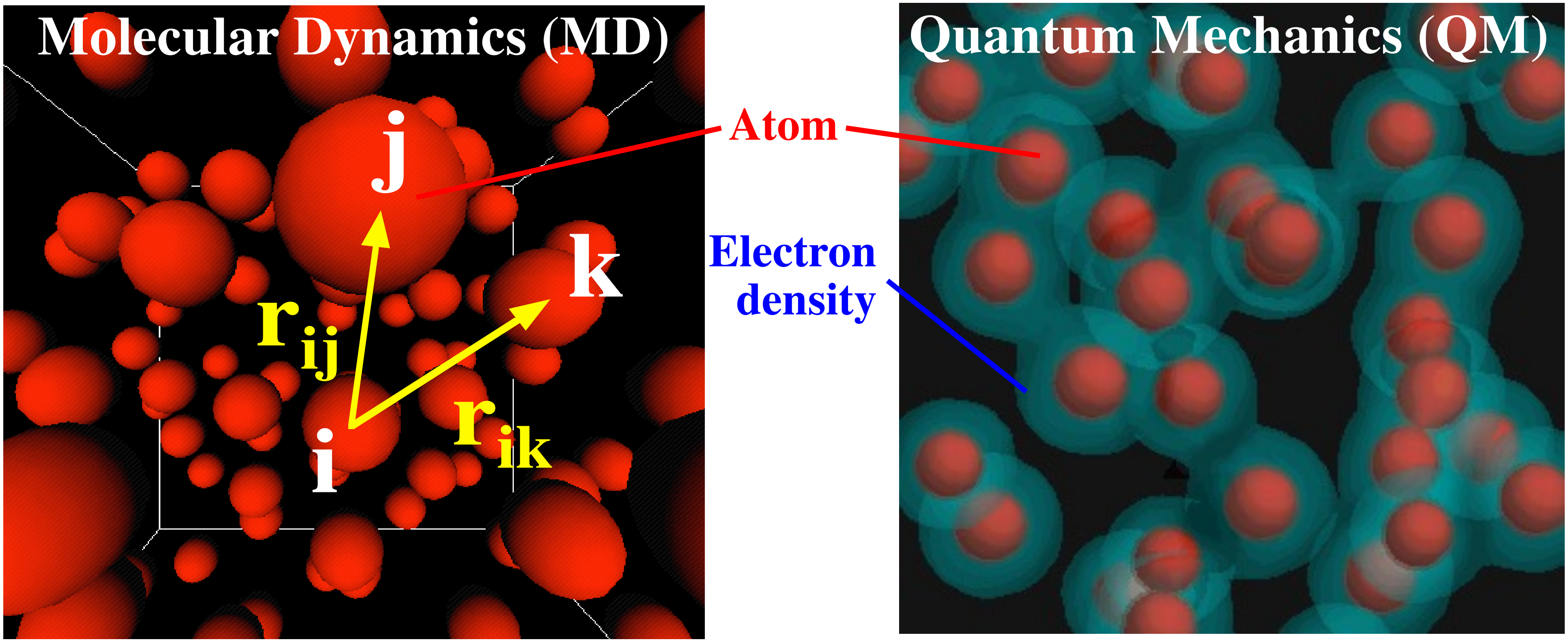
- Grid service description & instances: Definition & execution
- Service state, metadata & introspection
- Naming & name resolution: Universal resource identifier (URI)
- Service life cycle: Instantiate & destruct
- Fault type: Standard base type for all fault messages
- Service groups: Represent & manage groups of services

OGSA Services

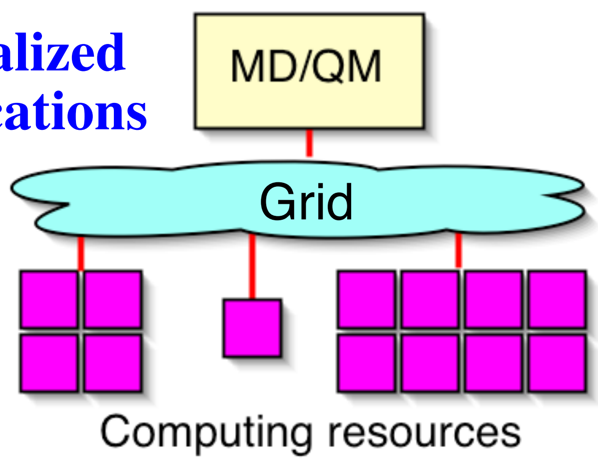
- Core services
  - Name resolution & discovery
  - Security
  - Policy
  - Messaging, queuing & logging
  - Events
  - Metering & accounting: Resource usage & charges
- Data & information services
  - Data management & access
  - Replication
  - Metadata & provenance
- Resource & service management
  - Provisioning & resource management
  - Service orchestration

Virtualization-aware Application Framework

Atomistic materials simulation methods



Virtualized applications



- Scalability
- Portable performance
- Adaptation

} → Data-locality principles
Divide-conquer-recombine

Research Issues

1. **Computational complexity:** Computation time, T, as a function of the problem size, N

   $O(N)$ < $O(N^m)$ < $O(C^N)$

   Easy ← Hard

2. **Scalability:** Parallel efficiency

   $$\eta = T_1/(T_p p) \sim 1$$

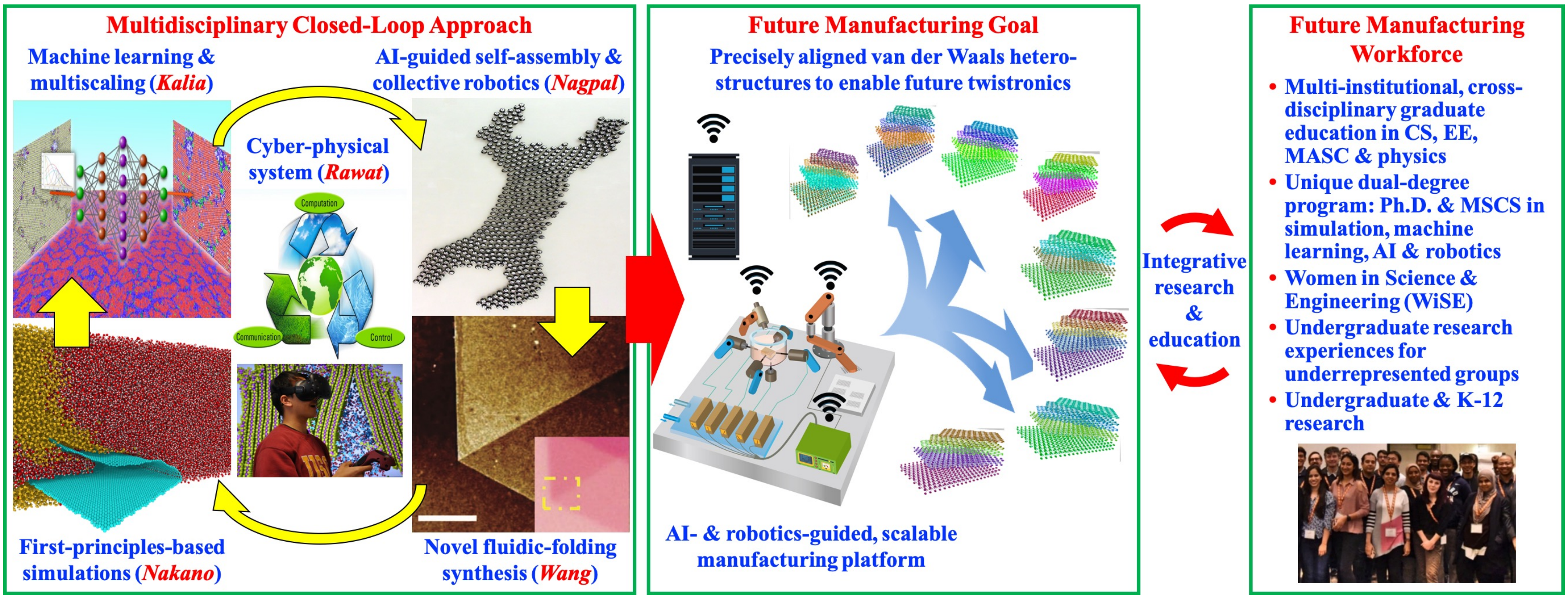
   for a large number, p, of processors

3. **Fault resilience**

Cybermanufacturing

NSF 2036359 FMRG: Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures

R. Nagpal (*Harvard*); R. Kalia, A. Nakano, H. Wang (*USC*); D. Rawat (*Howard*)



This project develops a transformative future manufacturing platform for quantum material architectures using a cybermanufacturing approach, which combines artificial intelligence, robotics, multiscale modeling, and predictive simulation for the automated & parallel assembly of multiple two-dimensional materials into complex three-dimensional structures.