Scientific Data Mining & Machine Learning

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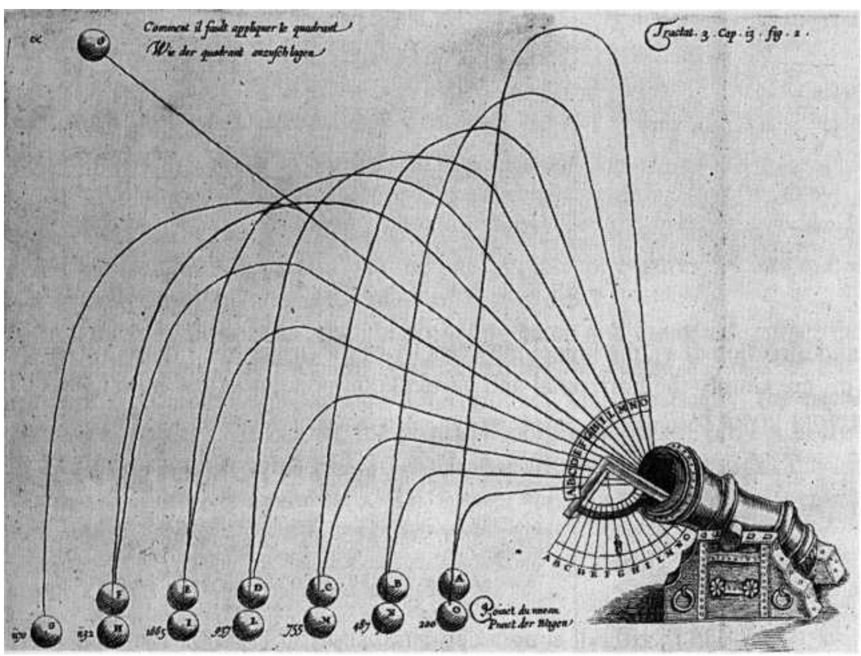
Scientific Data Mining

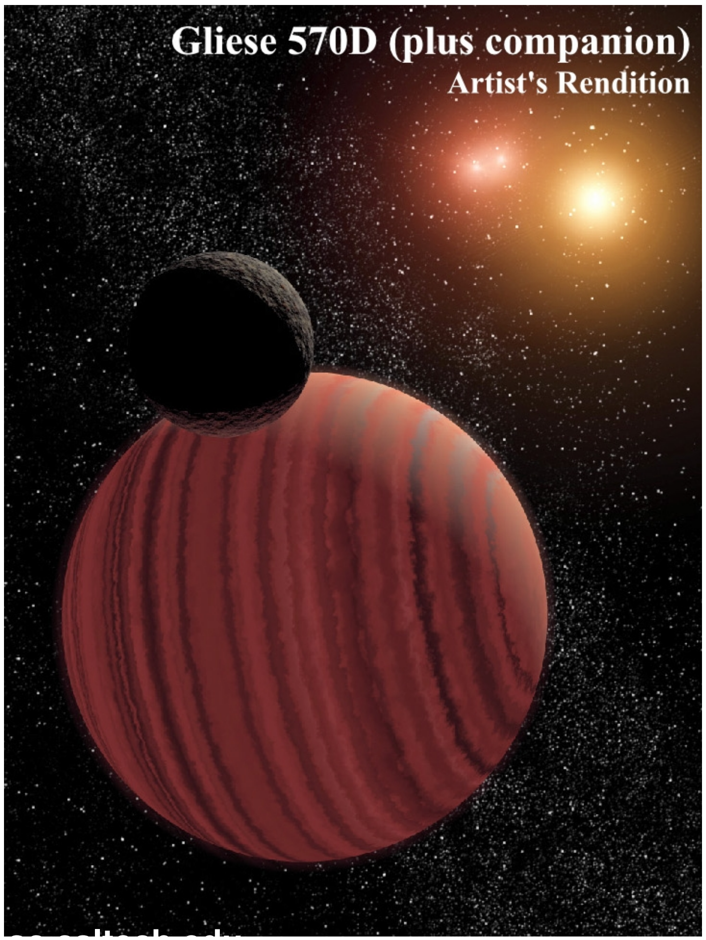
- **Scientific data mining: Automated detection of knowledge hidden in large & often noisy scientific (experimental, simulation, *etc*.) datasets**
- **Knowledge: Simplest (*i.e.*, minimal description length) explanation to replace exhaustive enumeration of the original data**

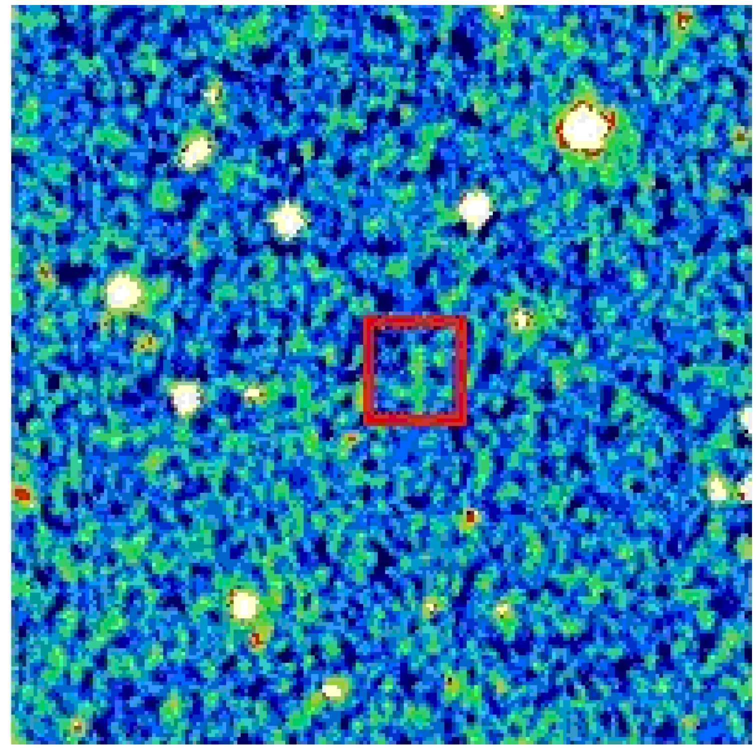


$$m\frac{d^2}{dt^2}\vec{r}(t) = \vec{F}$$

Google Science in the Flat World

Parallel computing on globally distributed supercomputers & visualization platforms will revolutionize & democratize science & engineering (*e.g.*, Google astronomy in the flat world)





SDSS image of brown dwarf, 2MASSI J0104075-005328

Atomistic Data as a Graph

- Molecular dynamics data
  - Atomic data: species, positions, velocities, stresses,…

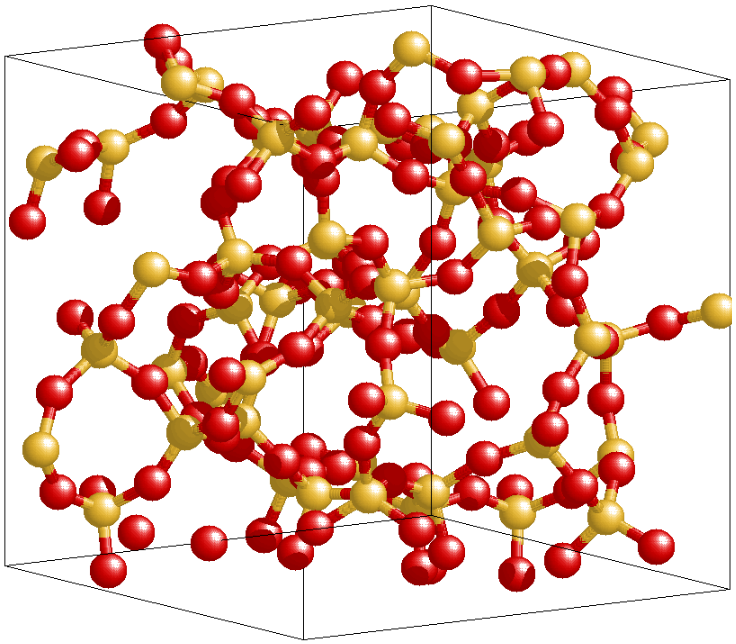
$$\{\lambda_i, \vec{r}_i, \vec{v}_i, \overleftrightarrow{\sigma}_i, \ldots | i = 1, \ldots, N\}$$

  - Atomic-pair data: bond order, pair distance,…

$$\left\{B_{ij}, \vec{r}_{ij}, \ldots \middle| i, j = 1, \ldots, N; i \neq j\right\}$$

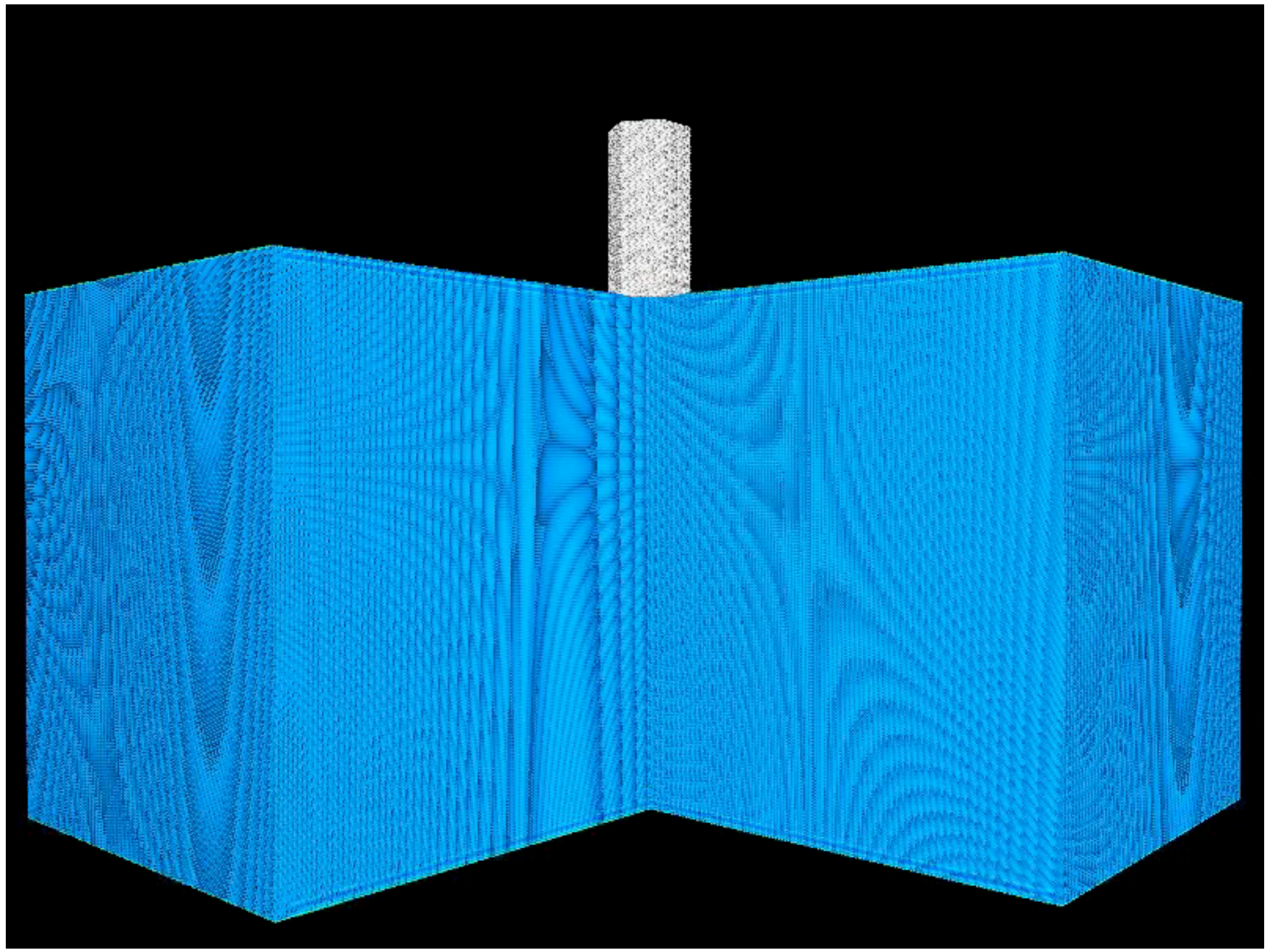
- Chemical bond network
  - Node degrees
  - Paths
  - Rings
  - Frequently occurring subgraphs

G = (*V*,*E*)
V: Set of atoms
E: Set of bonds



Hypervelocity Impact on Ceramics

- 209M-atom MD of AlN
- 300M-atom MD of SiC
- 540M-atom MD of Al_2O_3



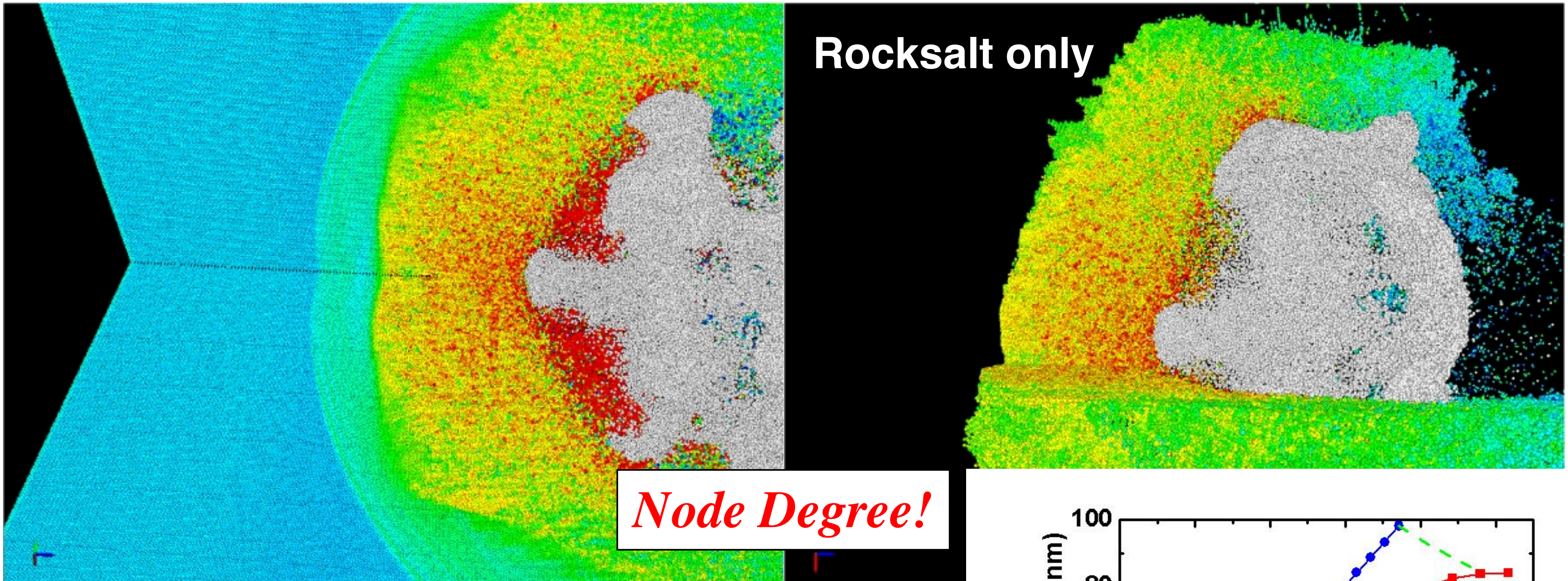
[0001]

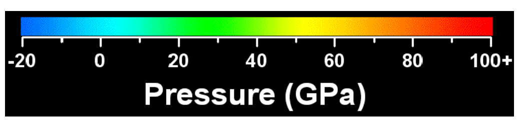
•Al_2O_3 plate

•18 km/s impact

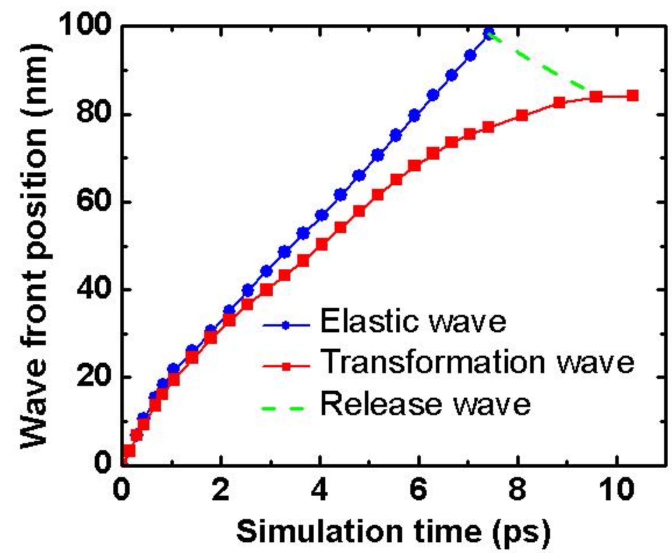
0.2μm

Shock-Induced Structural Phase Transformation in AlN

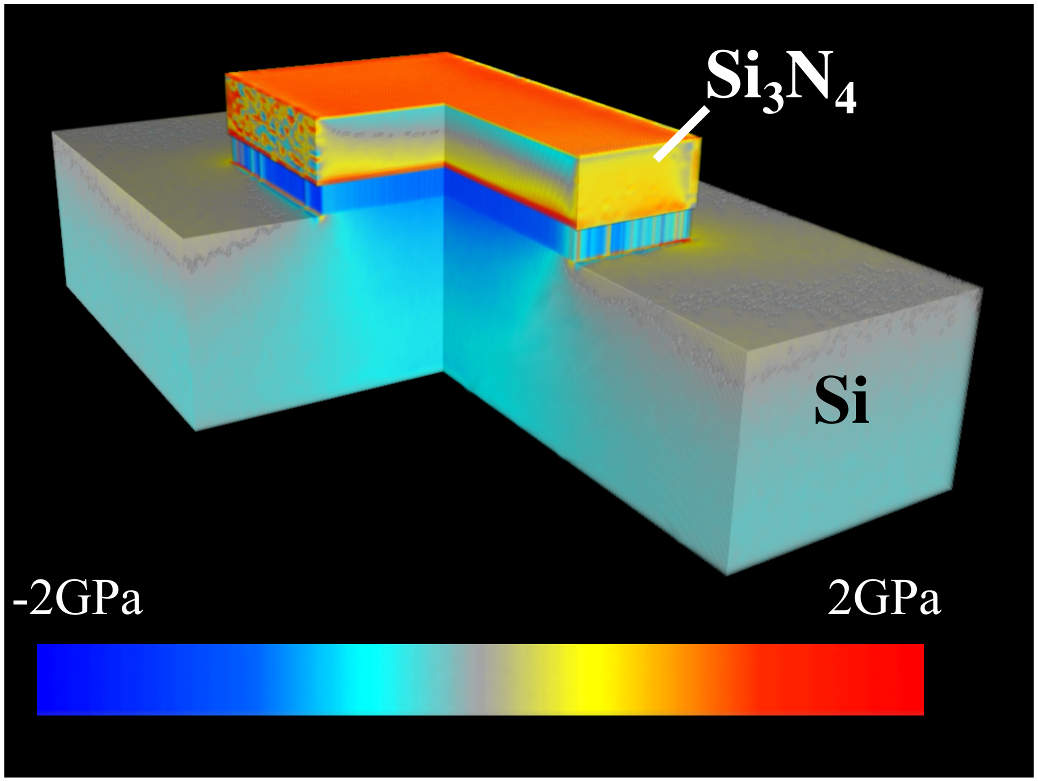


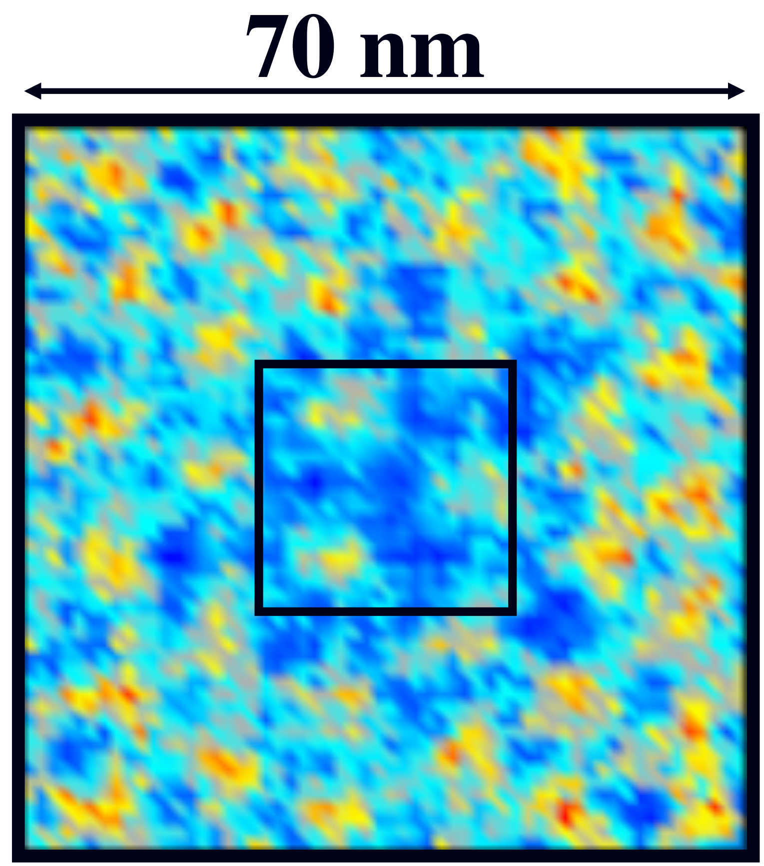


- Wurtzite (4-coordinated) to rocksalt (6-coordinated) phase transformation at 20 GPa



Stress Domains in Si_3N_4/Si Nanopixels

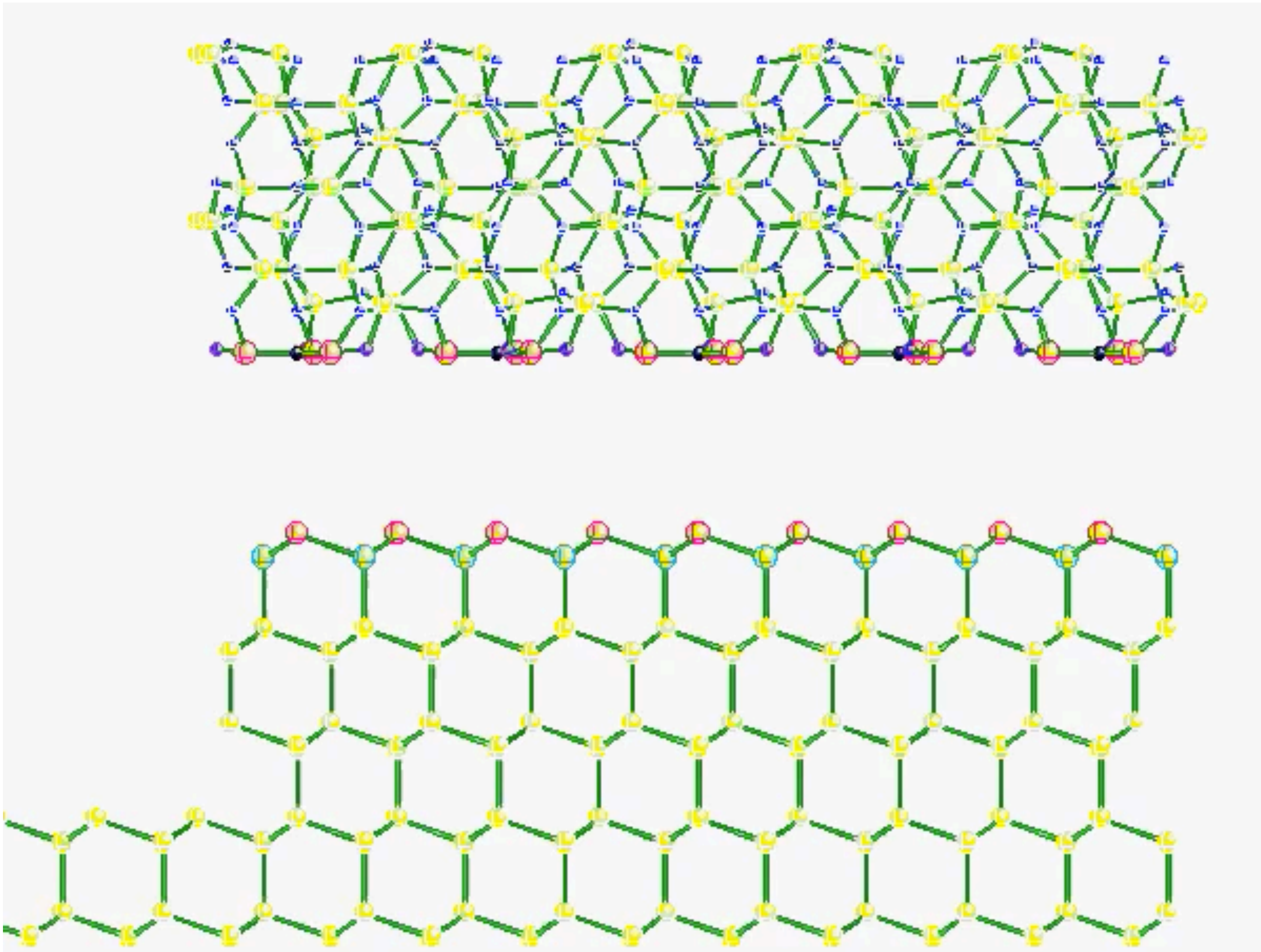




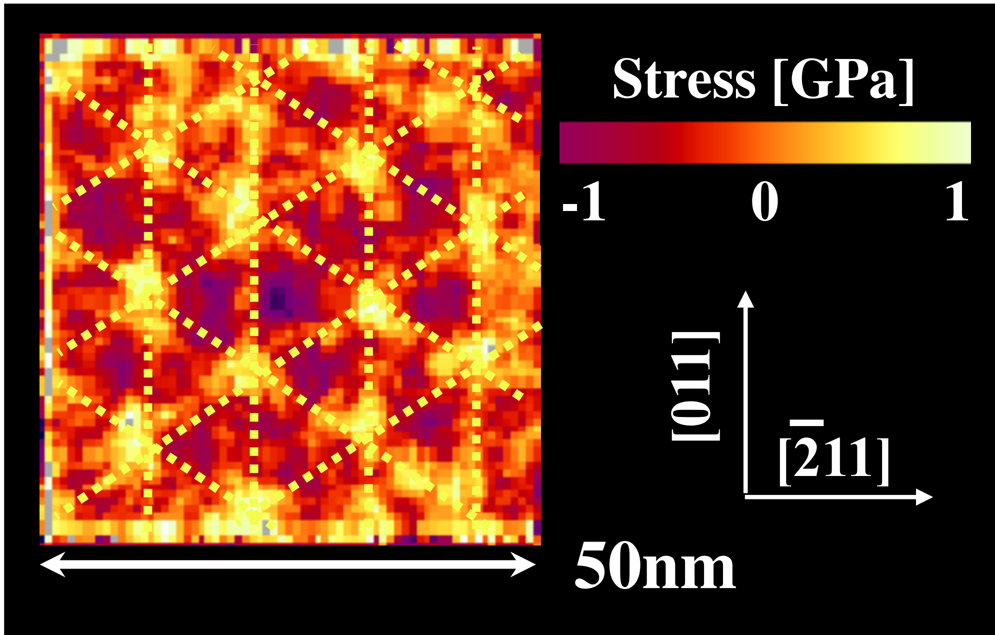
Stress well in Si with a crystalline Si_3N_4 film due to lattice mismatch

Stress domains in Si due to an amorphous Si_3N_4 film

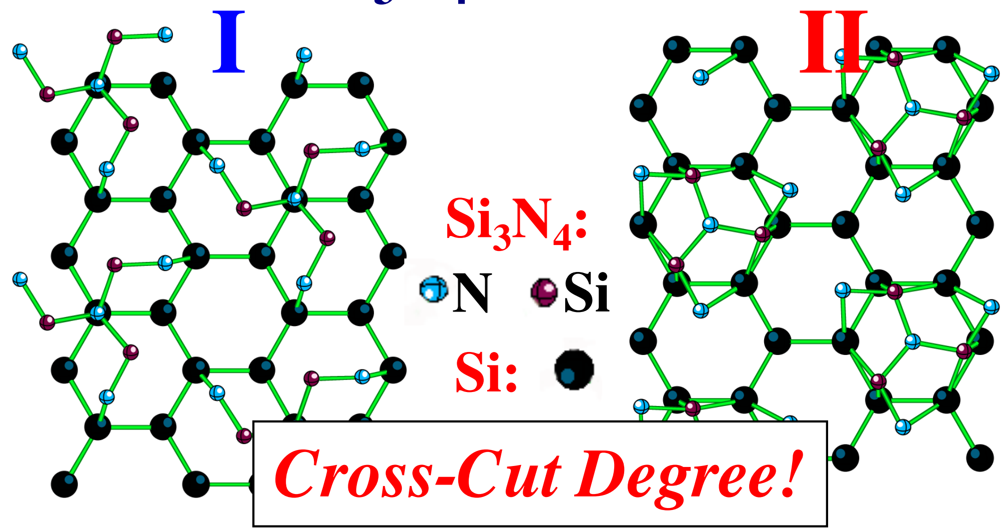
Si(111)/Si_3N_4(0001) Interface

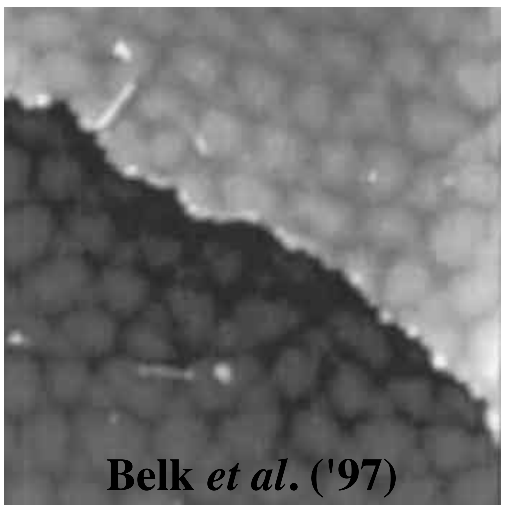


Stress Domains in Si/Si_3N_4 Nanopixel

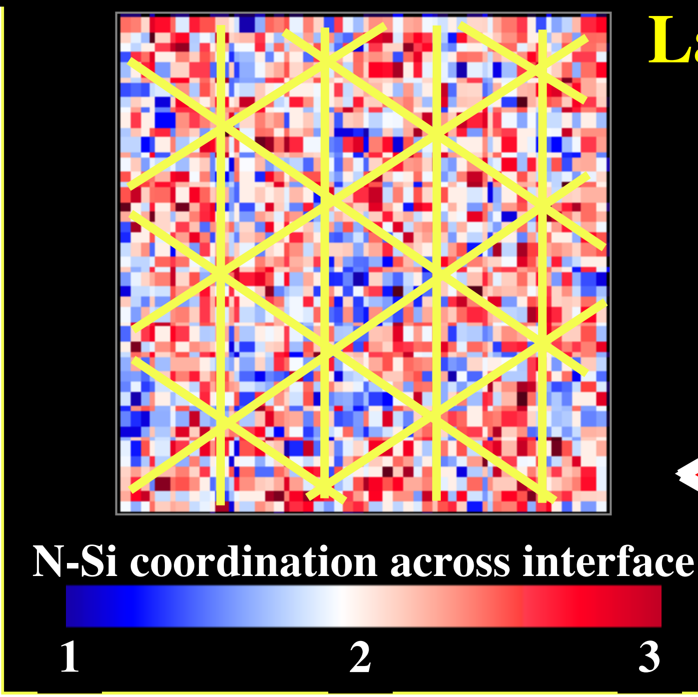


Si(111)/Si_3N_4(0001) interfaces

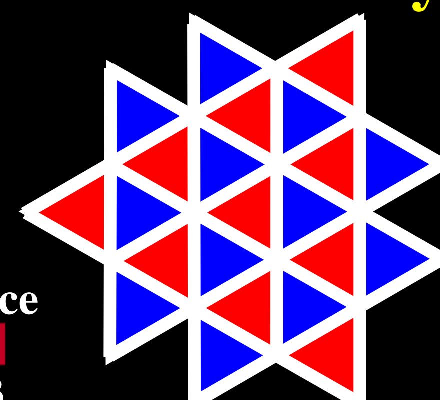




Misfit dislocation network in InAs/GaAs(111)

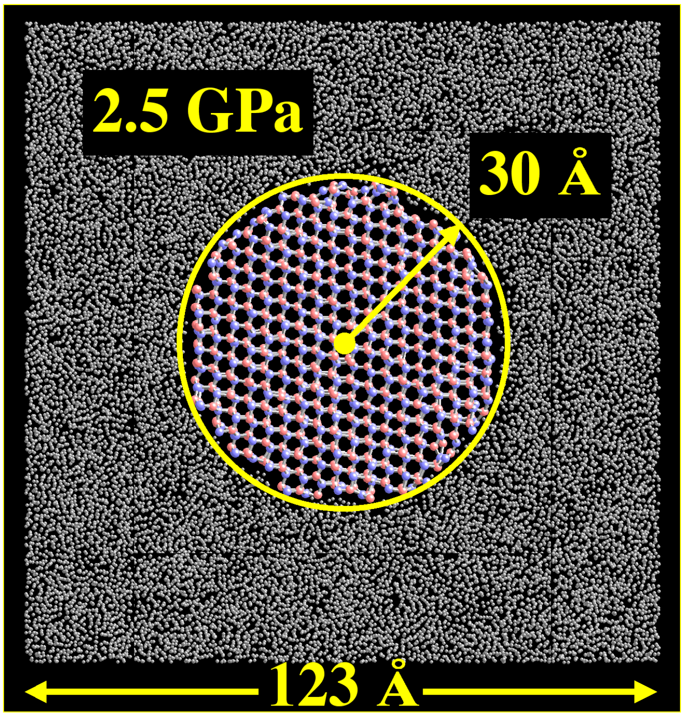


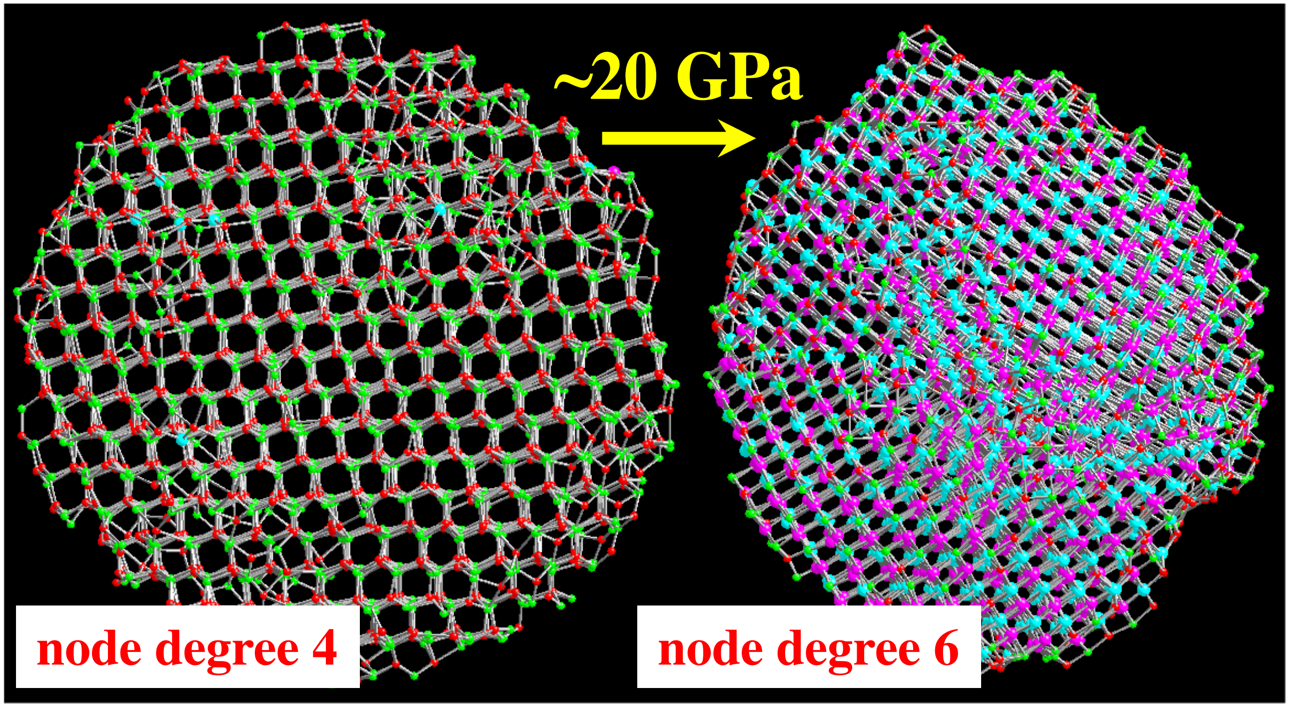
Lattice mismatch (1%) induced interfacial domain array



High-Pressure Structural Transformation

- Wurzite (node degree 4) to rocksalt (node degree 6) structural transformation of a GaAs nanoparticle under high pressure

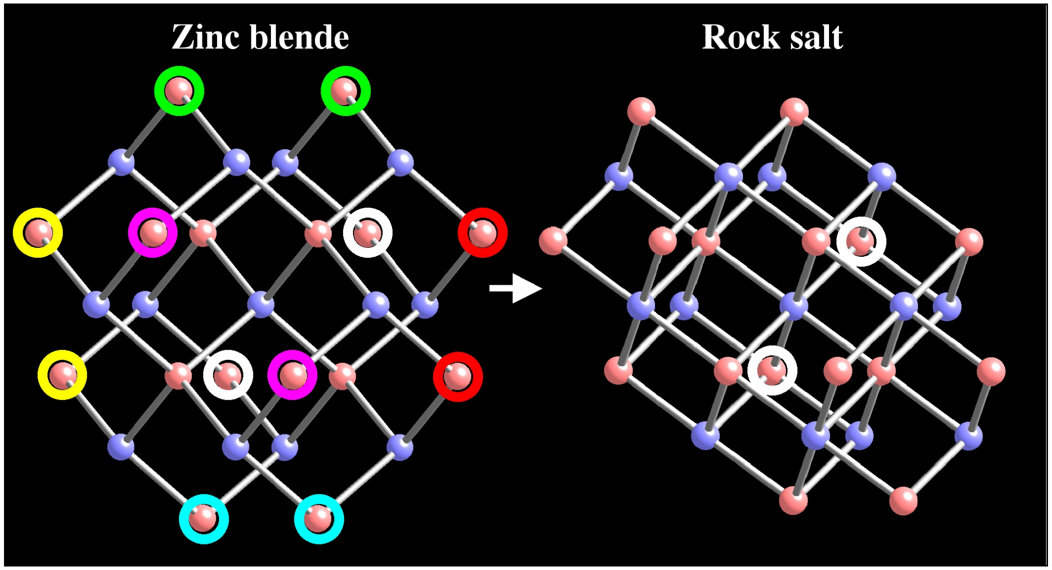


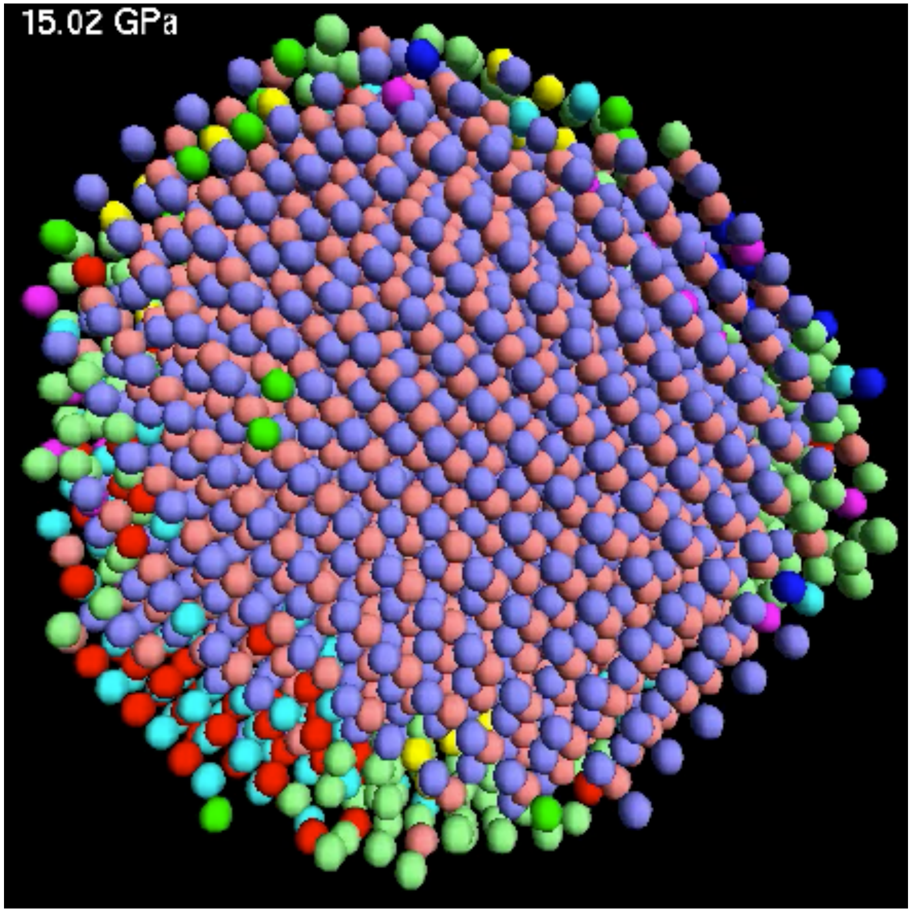


- Existence of multiple domains?

Graph-Transition Tracking

- **Finite set of graph transitions as a classifier**





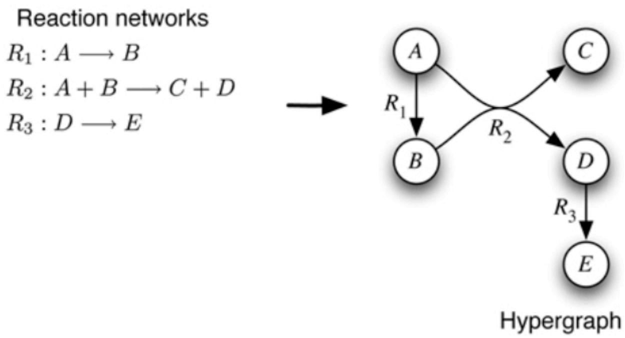
$$G = (V, E)$$
$$\downarrow$$
$$G' = (V, E')$$

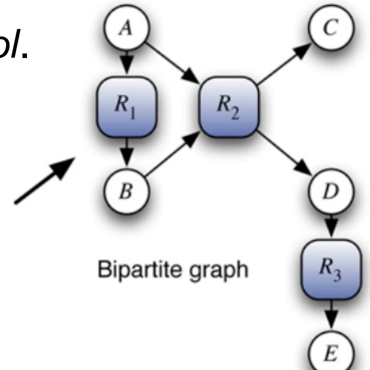
$$E \subset E'$$

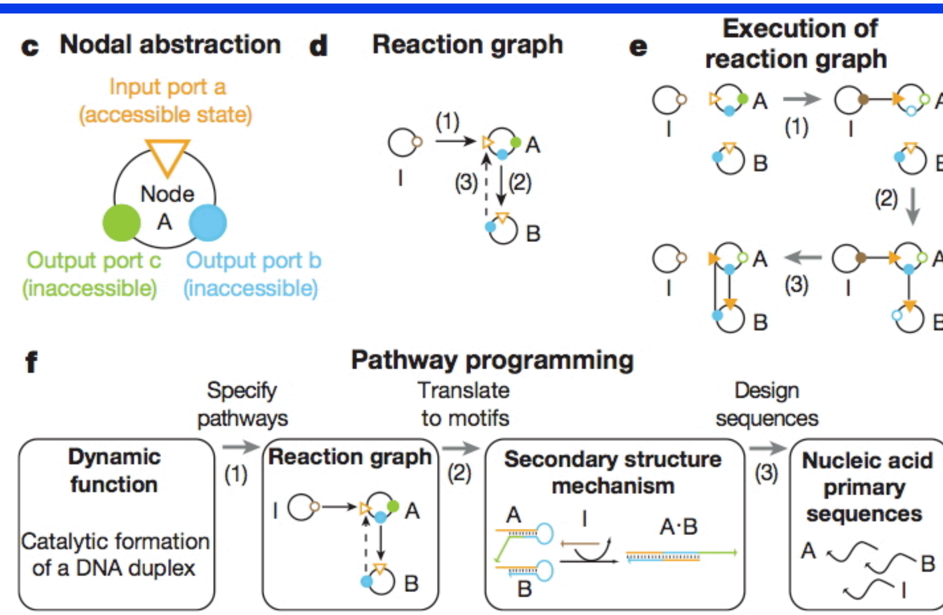
Graph Transition!

Chemical Reaction Network

Klamt *et al.*, *PLoS Comput. Biol.* **5**, e1000385 ('09)

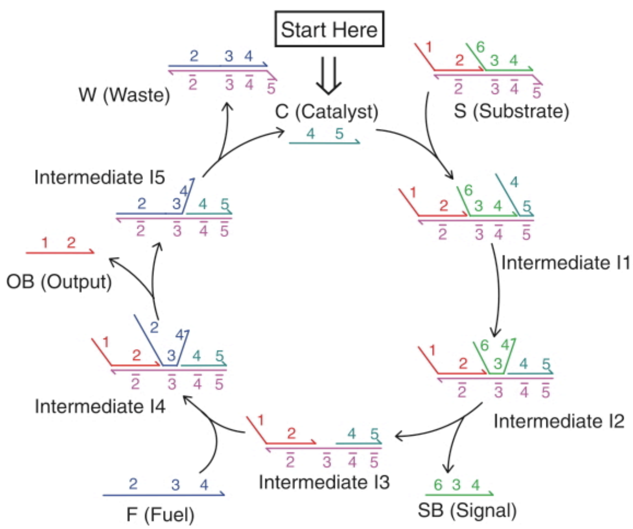


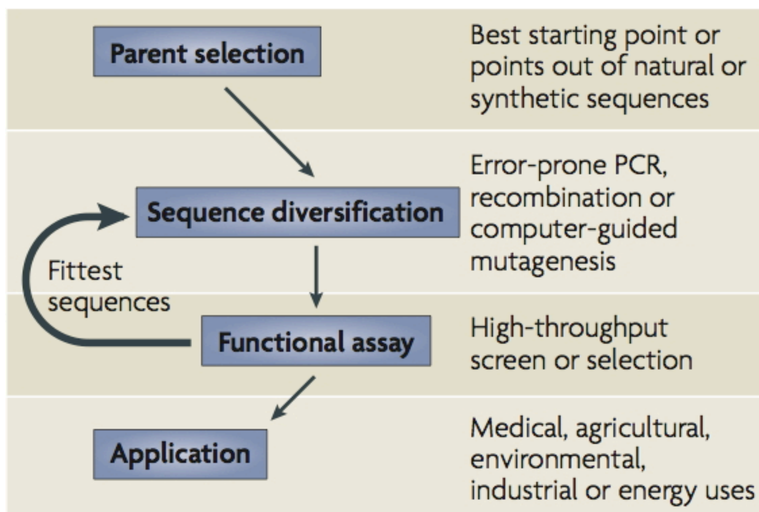


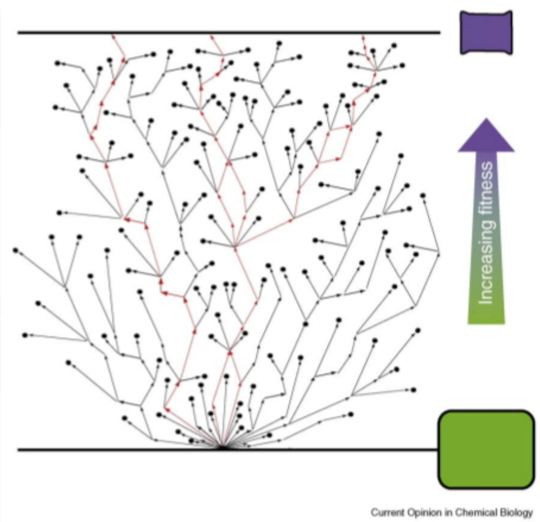


Yin *et al.*, *Nature* **451**, 318 ('08)

Zhang *et al.*, *Science* **318**, 1121 ('07)







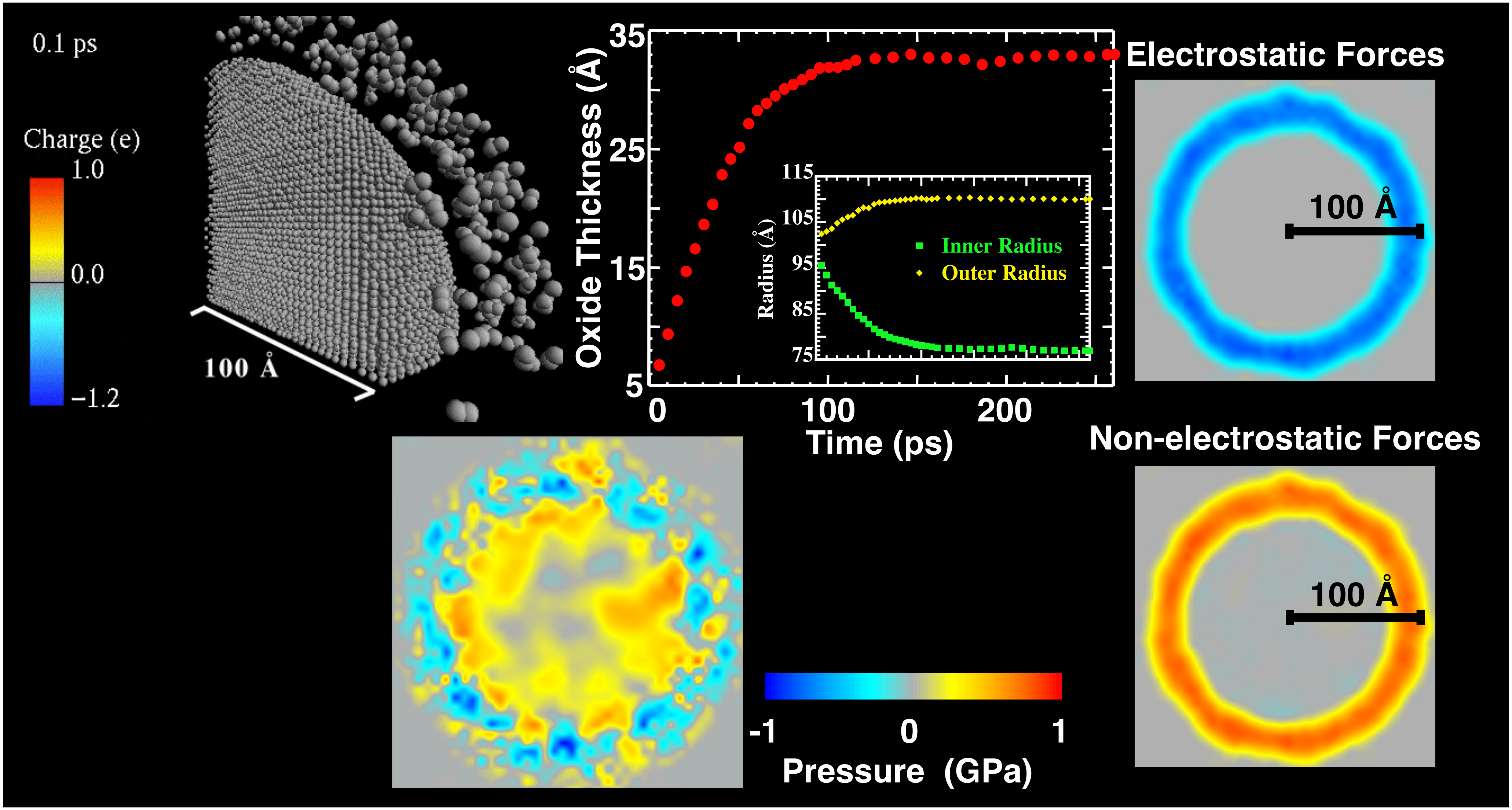
Arnold group, *Nature Rev. MCB* **10**, 867('09); *COCB* **13**, 3 ('09)

Reaction graph = language for self-assembly & catalytic cycle design

Directed & accelerated evolution

Chen *et al.*, *Nature Nanotechnol.* **8**, 755 ('13)

Oxidation of an Al Nanoparticle (n-Al)

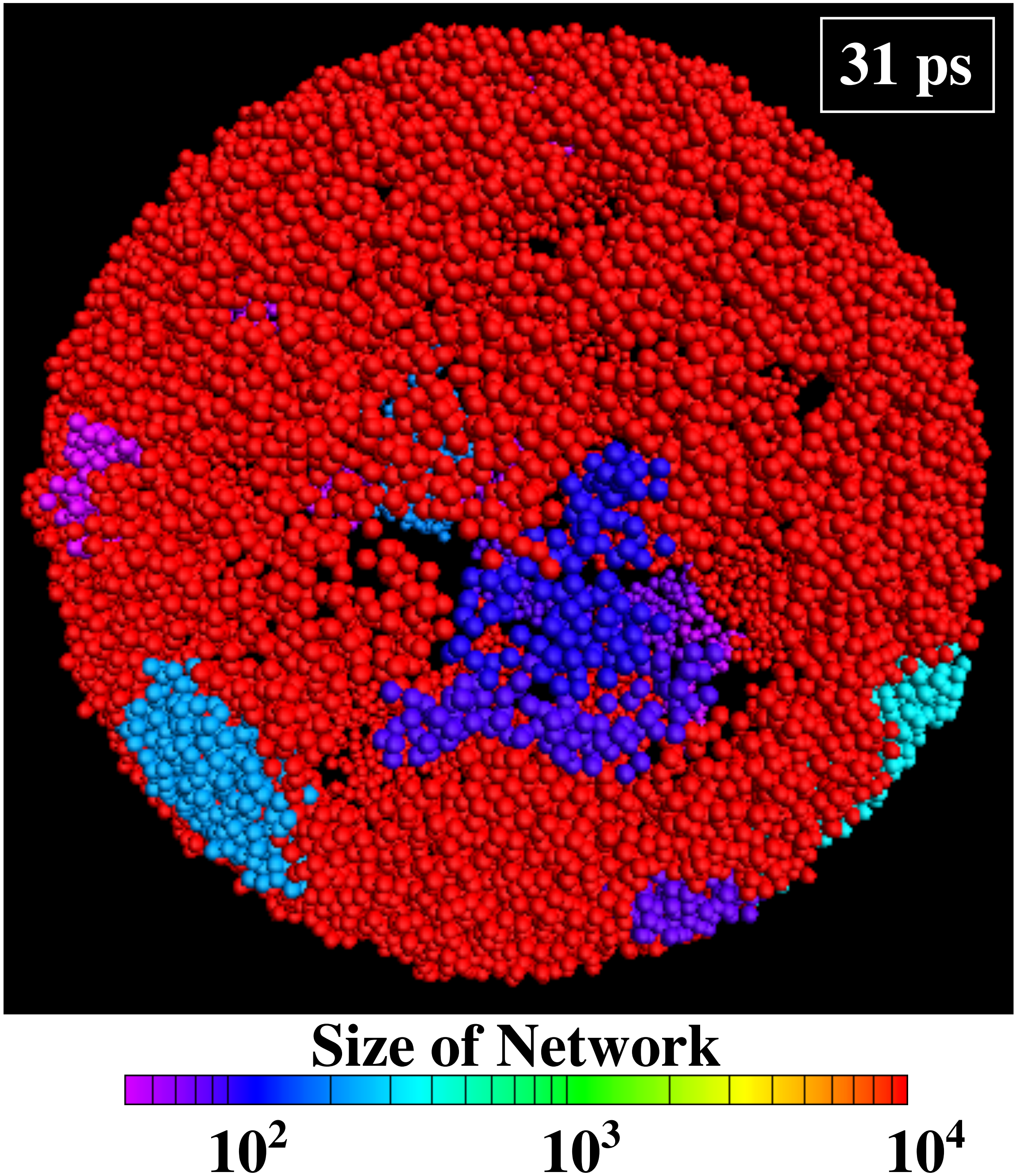


- Oxide thickness saturates at 40 Å after 0.5 ns, in agreement with experiments
- Oxide region/metal core is under negative/positive pressure
- Attractive Al-O Coulomb forces contribute large negative pressure in the oxide

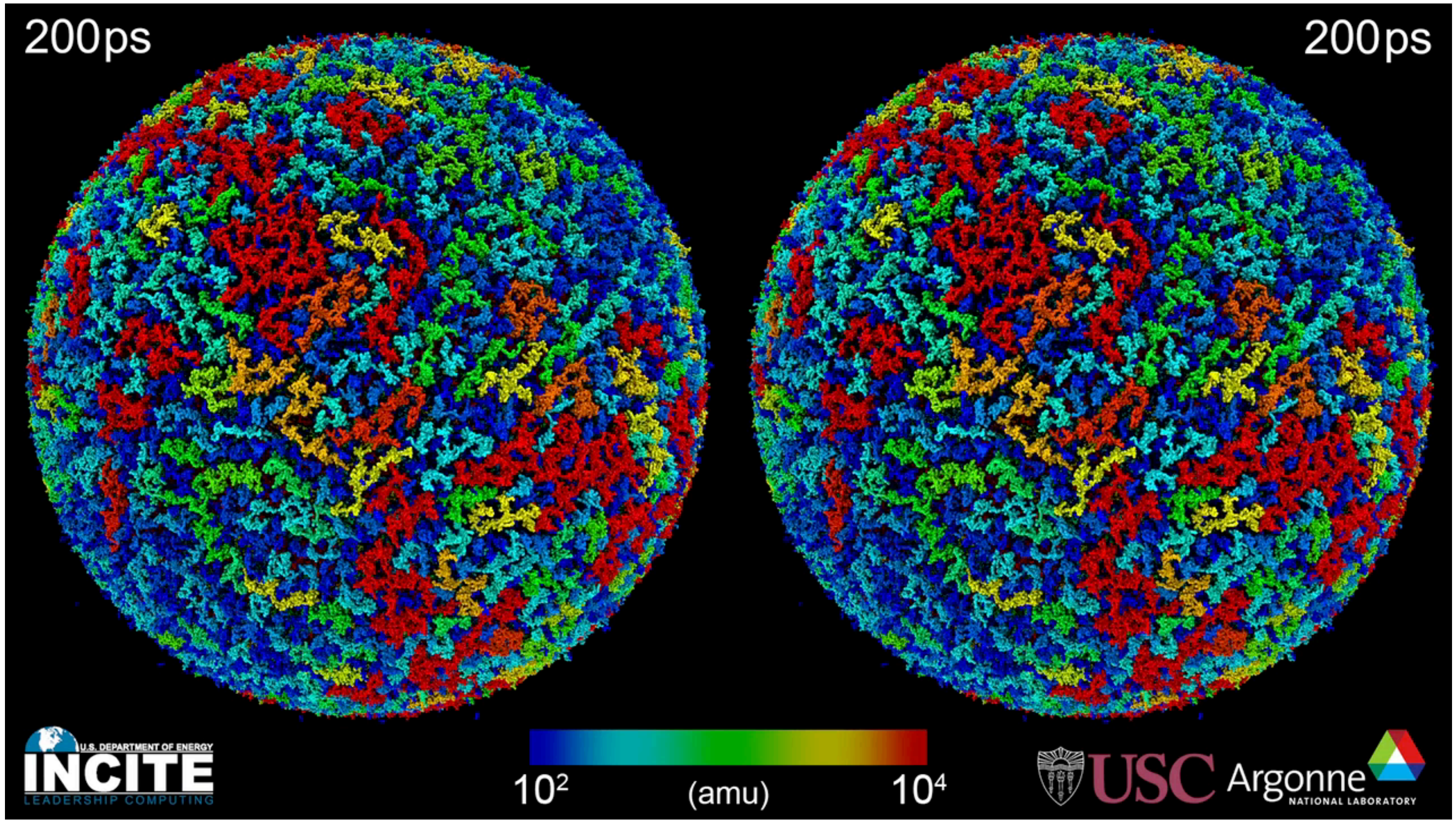
Oxidative Percolation

Clusters of OAl_4 coalesce to form a neutral, percolating tetrahedral network that impedes further growth of the oxide

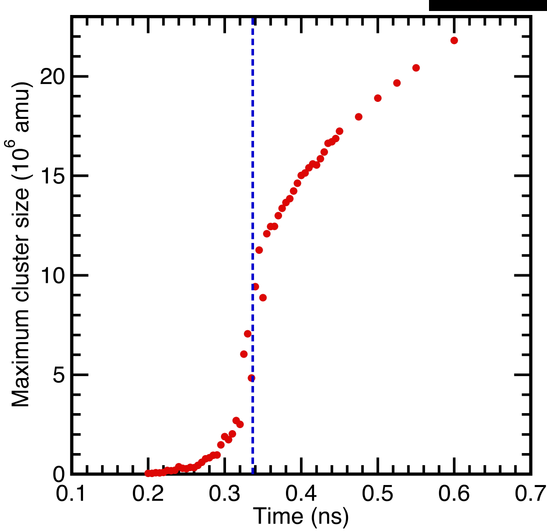
Percorative Connected Components!



Fractal Nanocarbon Product

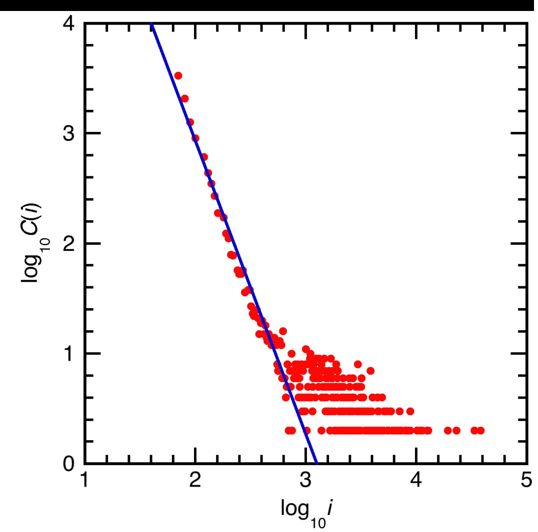


- **Percolation transition causes carbon clusters to exhibit power-law distribution of sizes: $C(i) \sim i^{-\tau}$**



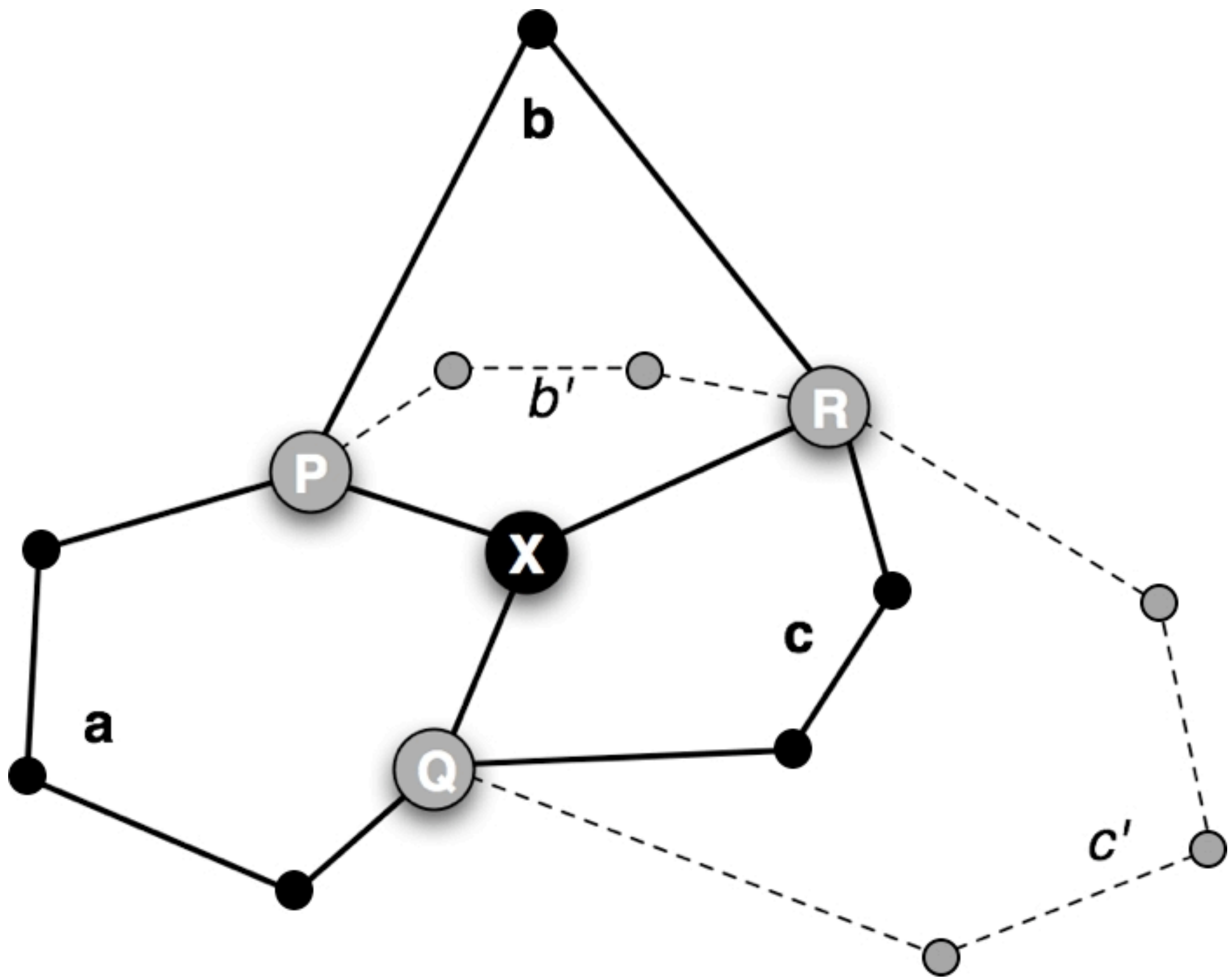
- **Fractal nanocarbon product with large surface areas may find supercapacitor, battery-electrode & mechanical metamaterial applications: $d_f = d/(\tau - 1) \sim 1.85$**

K. Nomura *et al*., *Sci. Rep*. **6**, 24109 ('16)
J. Insley *et al*., *IEEE/ACM SC16*



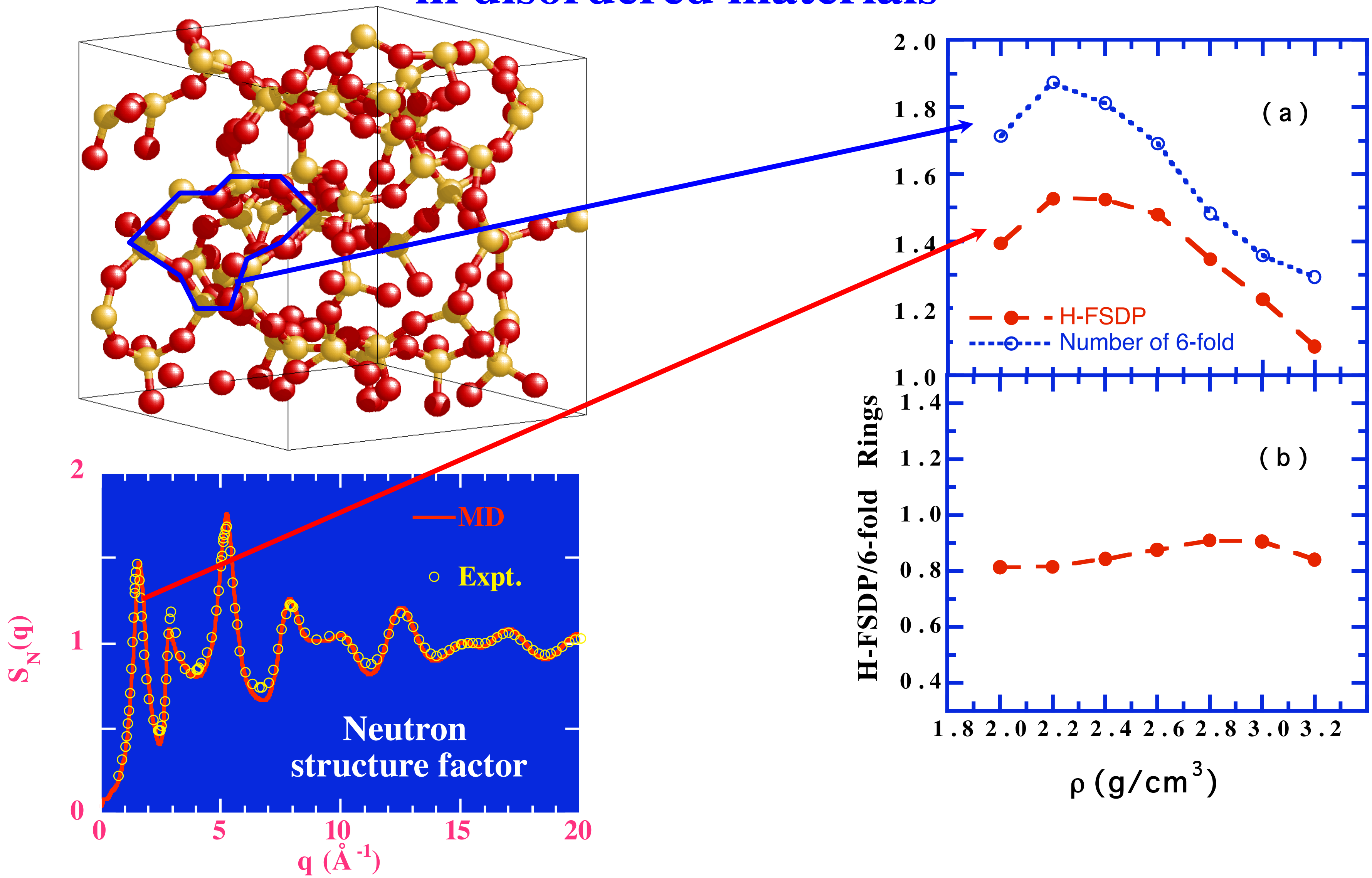
Shortest-Path Rings

- **K-ring:** Given a vertex x & two of its neighbors w & y, a K-ring generated by the triplet w–x–y is any ring containing the edges [w–x], [x–y] and a shortest path w–y path in G–x



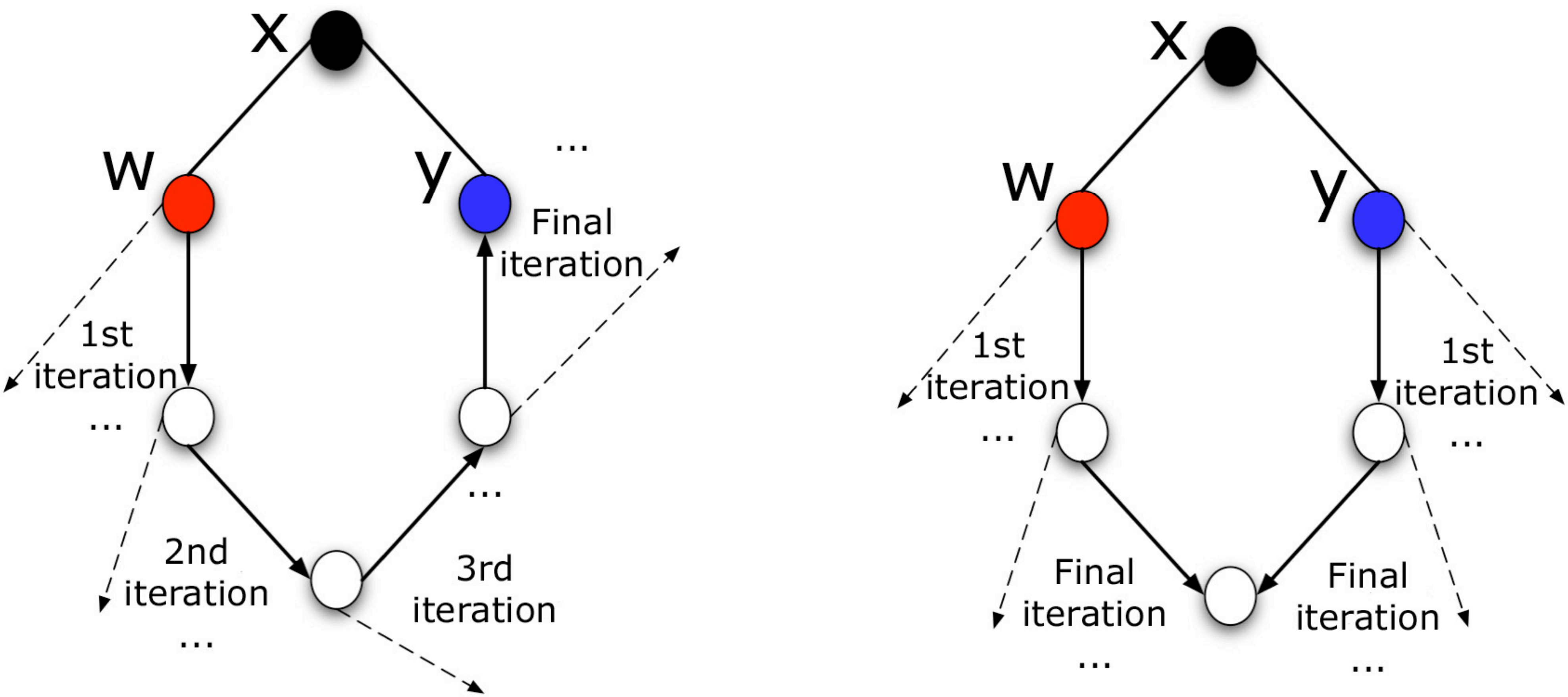
Ring-based Data Mining

Shortest-path ring analysis of intermediate-range order (IRO) in disordered materials



Correlation between IRO in neutron scattering & ring distribution

Fast Ring Analysis: Dual-Tree Expansion



Original Algorithm

Proposed Algorithm

C. Zhang *et al.*, *Computer Physics Communications* **175**, 339 ('06)

DTE Algorithm

Algorithm dual_tree_expansion()

Input:

V = Set of all vertices (i.e., atoms)
R_c = Ring cutoff range (Euclidean)
R_{bc} = Bond cutoff distance (Euclidean)
L_{MAX} = Maximum length of ring (integer)
P = Number of compute nodes

Output:

The K-ring statistics for all vertices in the network
List of atoms with abnormal ring profile

Variables:

Neighbors(V) = Set of vertices that share an edge with vertex V
$K_v(p)$ = Number of p-member rings that go through vertex V
L_{ij} = Length of the ring formed with path (V_i, V, V_j)

Steps:

0 coarse grained spatial decomposition of atoms on P compute nodes with a thin boundary extension of R_c distance (This step is for the parallel version only)
1 create adjacency list G for all node in V_p using R_{bc} as cutoff distance
2 for every vertex $V \in V_p$
    for each vertex pair V_i and V_j in Neighbors(V) do
        $A_1 = \{V_i\}$
        $A_2 = \{V_j\}$
        $L_{ij} = 0$
        while ($A_1 \cap A_2 = \varnothing$ AND $L_{ij} < L_{MAX}$) do
            $L_{ij} = L_{ij} + 2$
            if ($A_1 \cap$ Neighbors(A_2) $\neq \varnothing$ OR $A_2 \cap$ Neighbors(A_1) $\neq \varnothing$)
                $L_{ij} = L_{ij} + 1$
                break
            else if (Neighbors(A_1) $\cap$ Neighbors(A_2) $\neq \varnothing$)
                $L_{ij} = L_{ij} + 2$
            A_1 = Neighbors(A_1)
            A_2 = Neighbors(A_2)
        if ($L_{ij} < L_{MAX}$) $++K_v(L_{ij})$

Spatial Hash-Function Tagging

Algorithm spatial hash function tagging (SHAFT)

Input:

$C(V)$ = 3D coordinates of all vertices (i.e., atoms)
R_c = Ring cutoff range (Euclidean)
R_{bc} = Bond cutoff distance (Euclidean)
L_{MAX} = Maximum length of ring (integer)

Output:

The integer index that is unique for all vertices in the maximum ring span

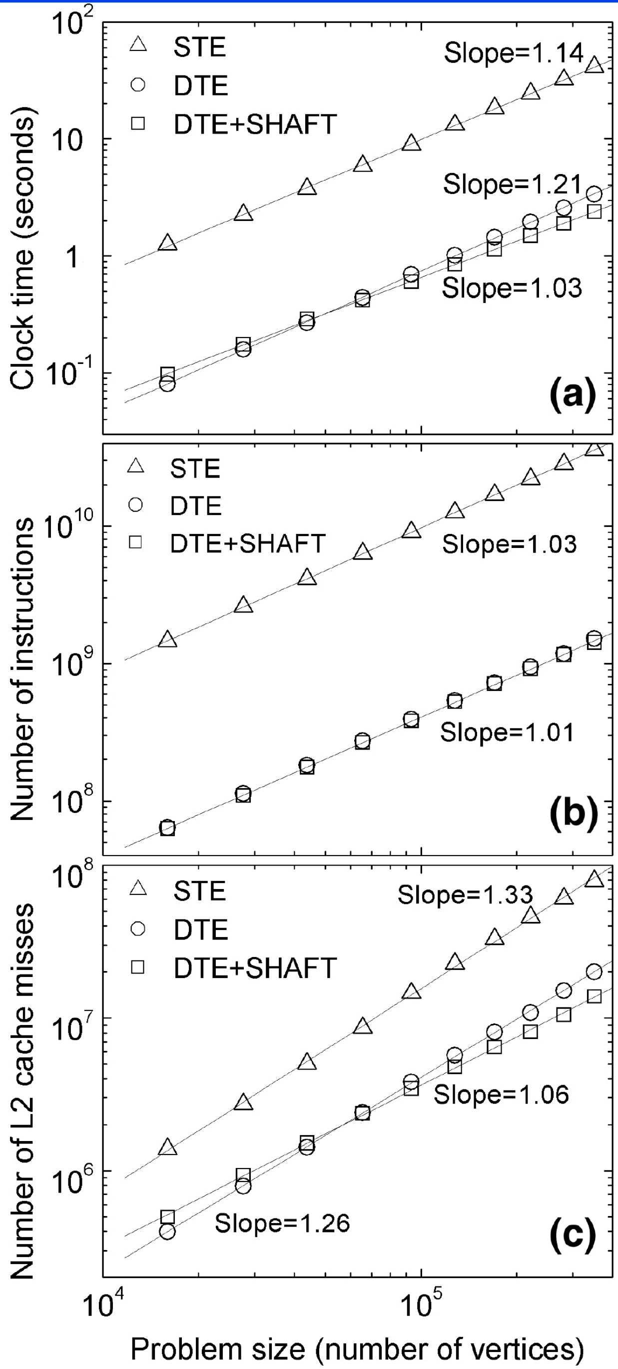
$b = R_{lower} / \sqrt{3}$
$c = R_{upper} L_{max}$
$m = \lceil c/b \rceil$

Step:

for each vertex
 for each spatial dimension i from 1 to 3
 $q_i = \lfloor C_i/b \rfloor$
 $q_i \,\% = m$
 return $q = q_3 \times m^2 + q_2 \times m + q_1$

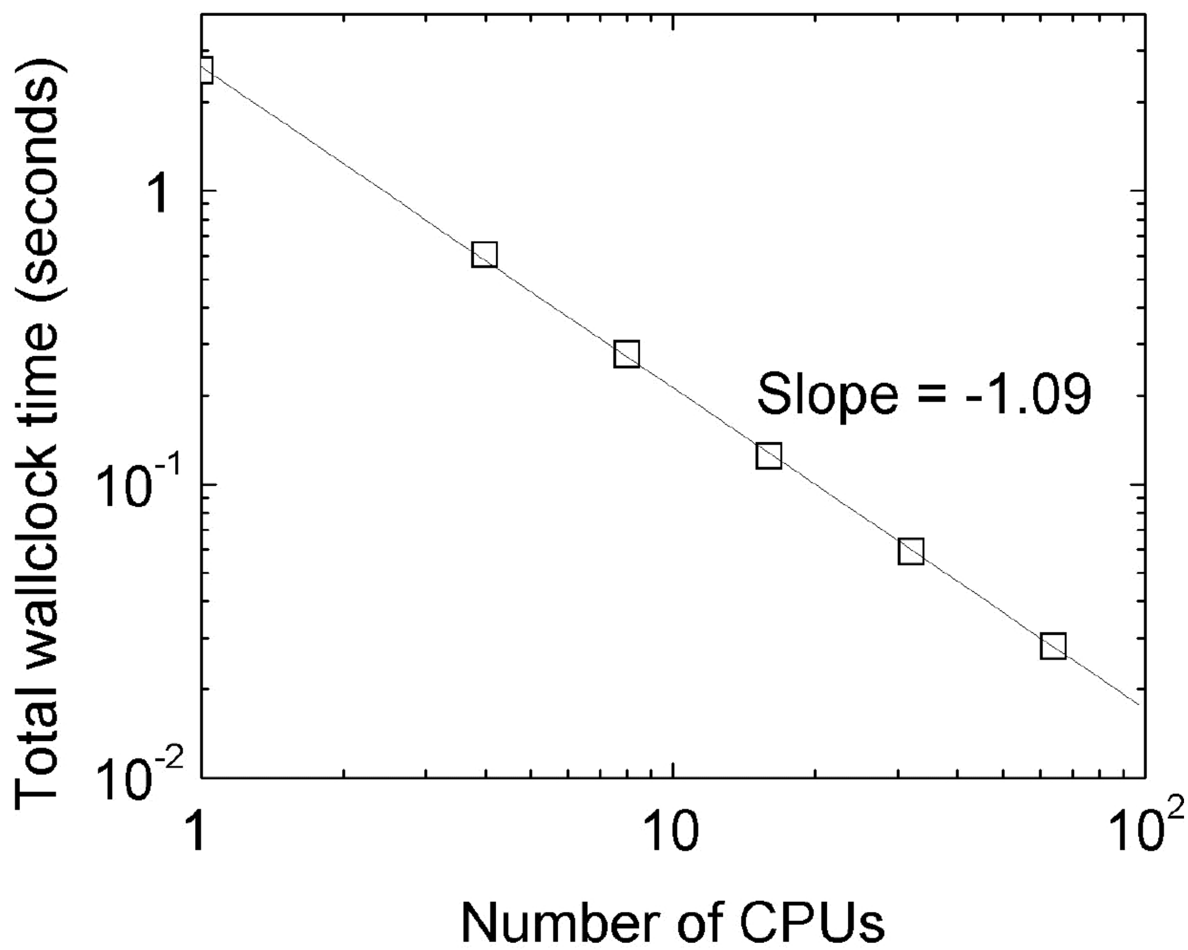
0	1	2	3	4	0	1	2	3	4
5	6	7	8	9	5	6	7	8	9
10	11	12	13	14	10	11	12	13	14
15	16	17	18	19	15	16	17	18	19
20	21	22	23	24	20	21	22	23	24
0	1	2	3	4	0	1	2	3	4
5	6	7	8	9	5	6	7	8	9
10	11	12	13	14	10	11	12	13	14
15	16	17	18	19	15	16	17	18	19
20	21	22	23	24	20	21	22	23	24

Numerical Tests



Linear scaling on the problem size

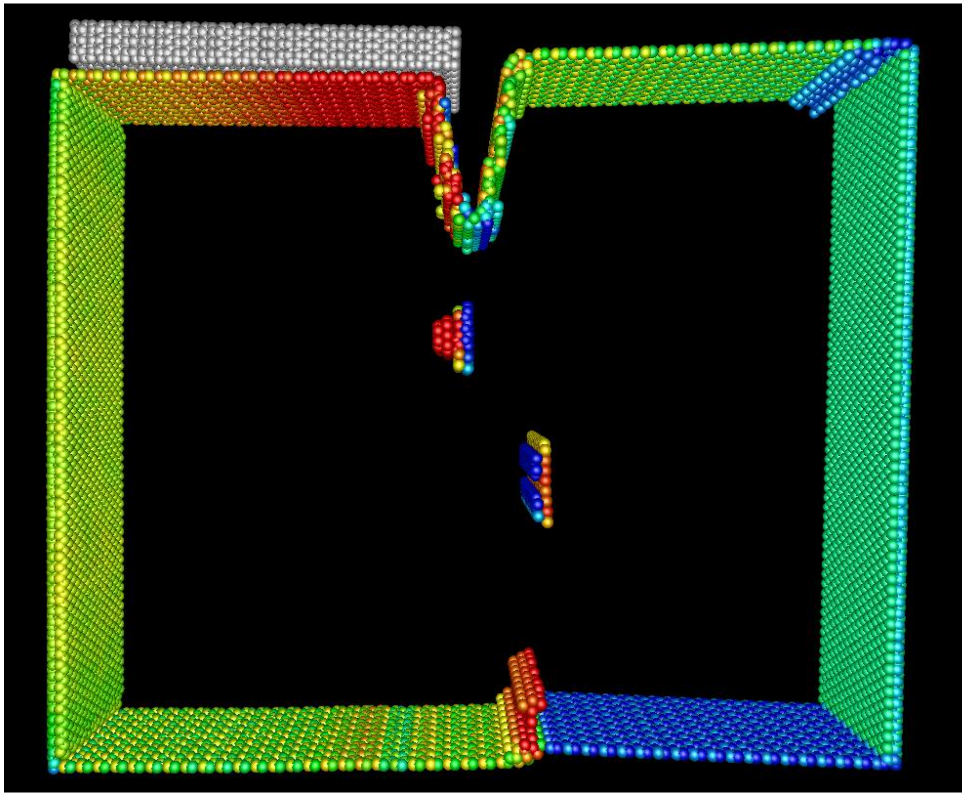
Superlinear (strong) scaling on the number of CPUs



Dislocation Mining

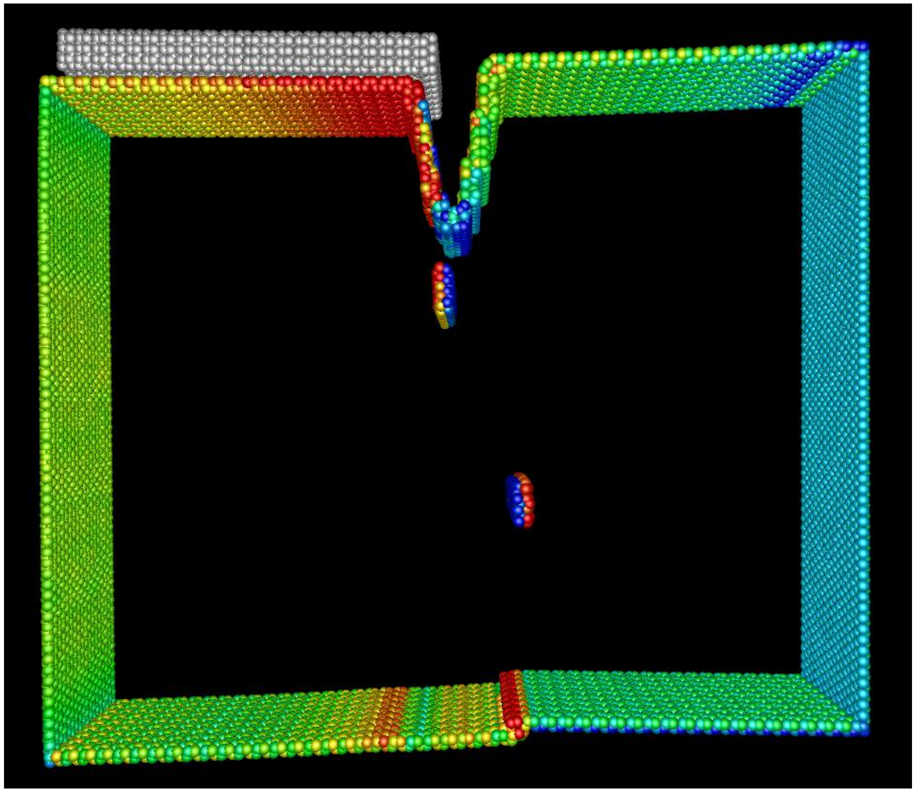
Based on potential energy

Shown atoms with high energy compared to bulk



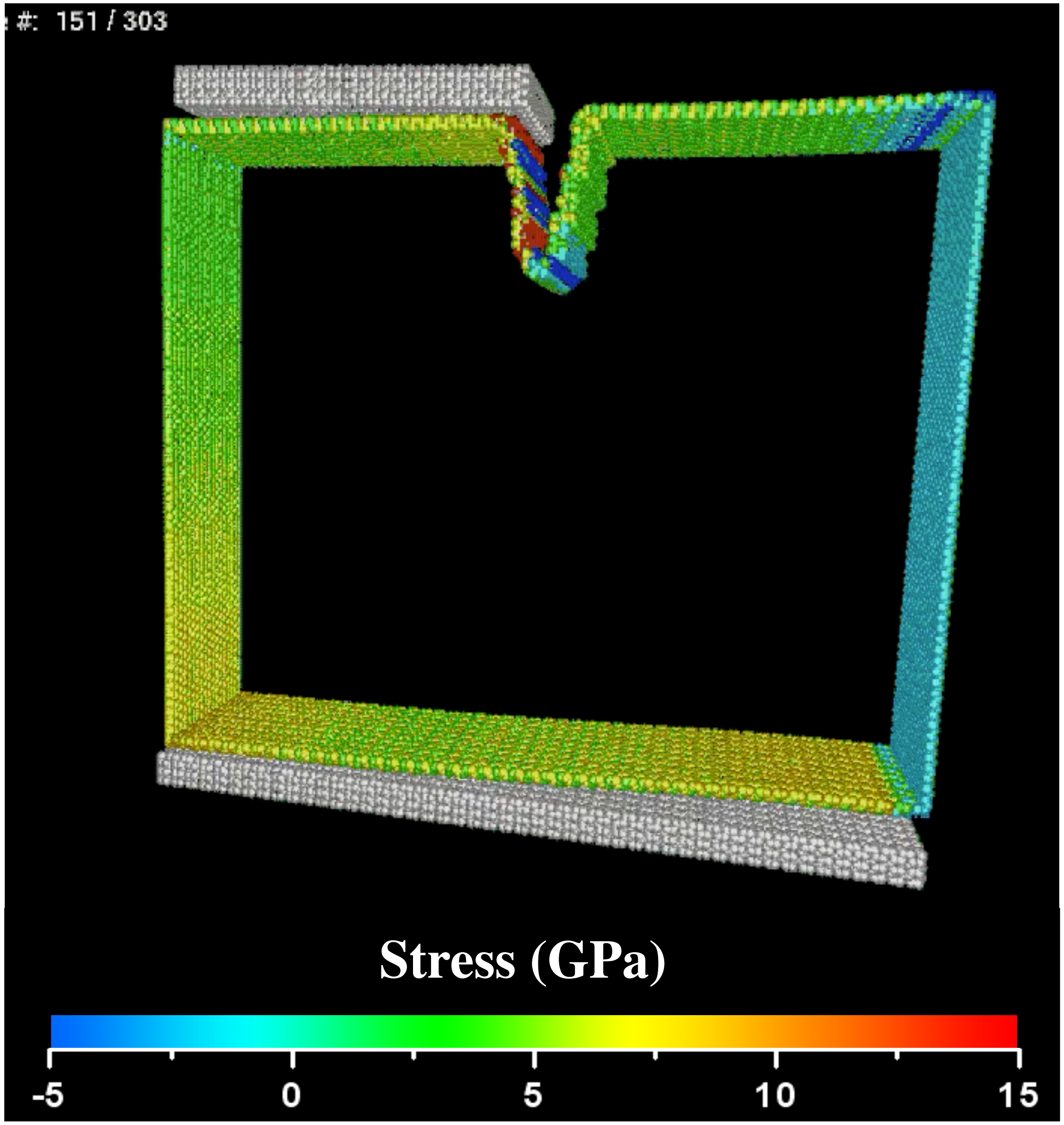
Based on shortest-path ring statistics

Shown atoms with less than 12 6-membered rings



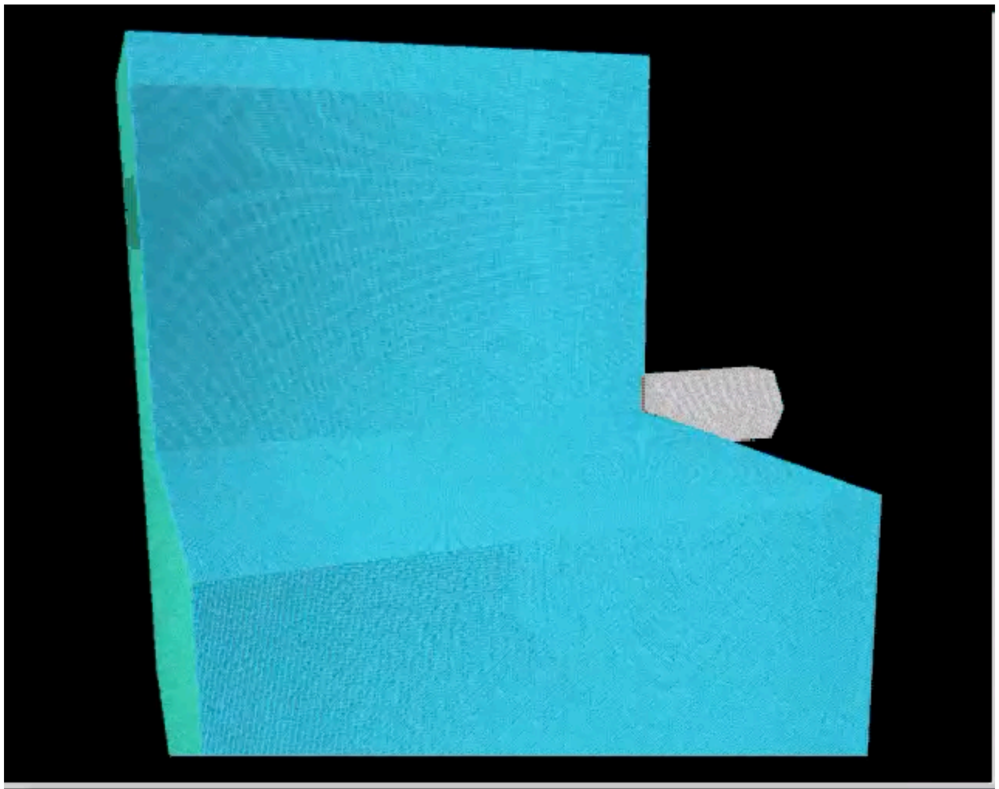
100 km/s Impact on Notched AlN

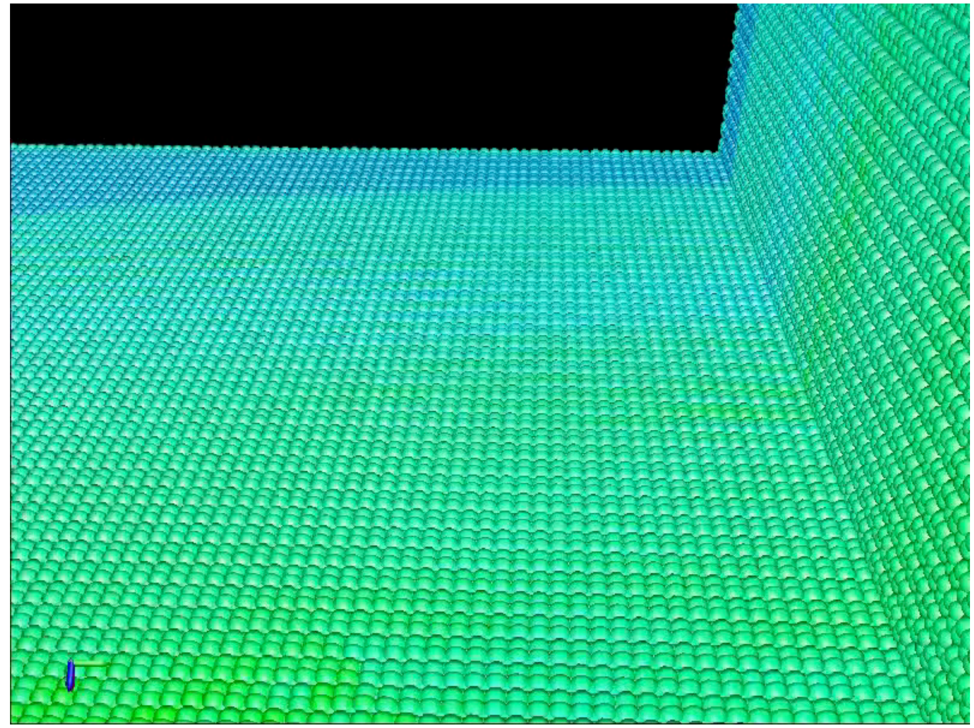
- Dislocation nucleation & emission from notch during impact
- Dislocations & surface atoms mined by ring statistics

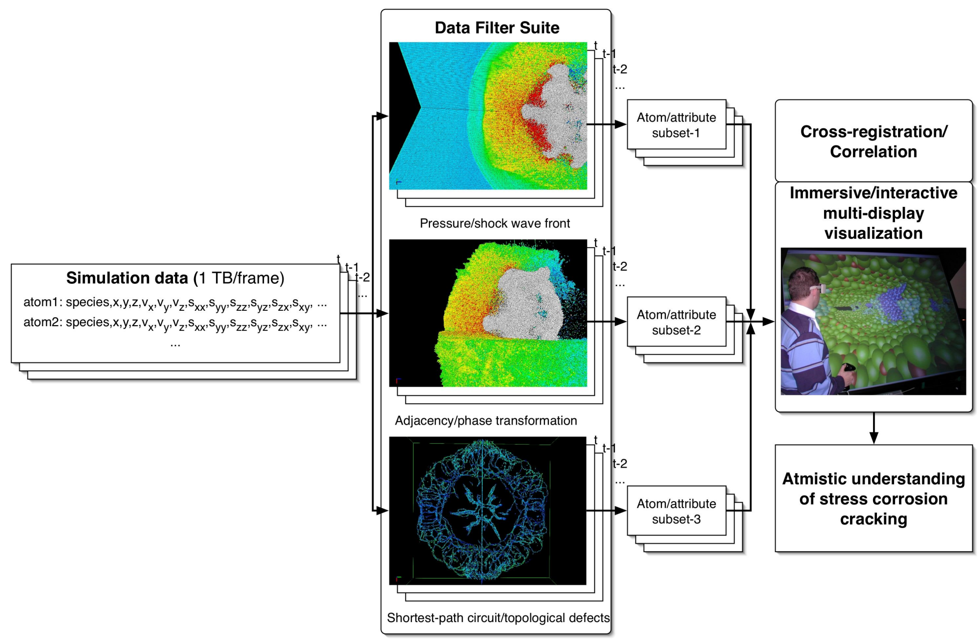


Impact-Damage Tolerant Ceramics?

Inverse problem: design materials with desired properties

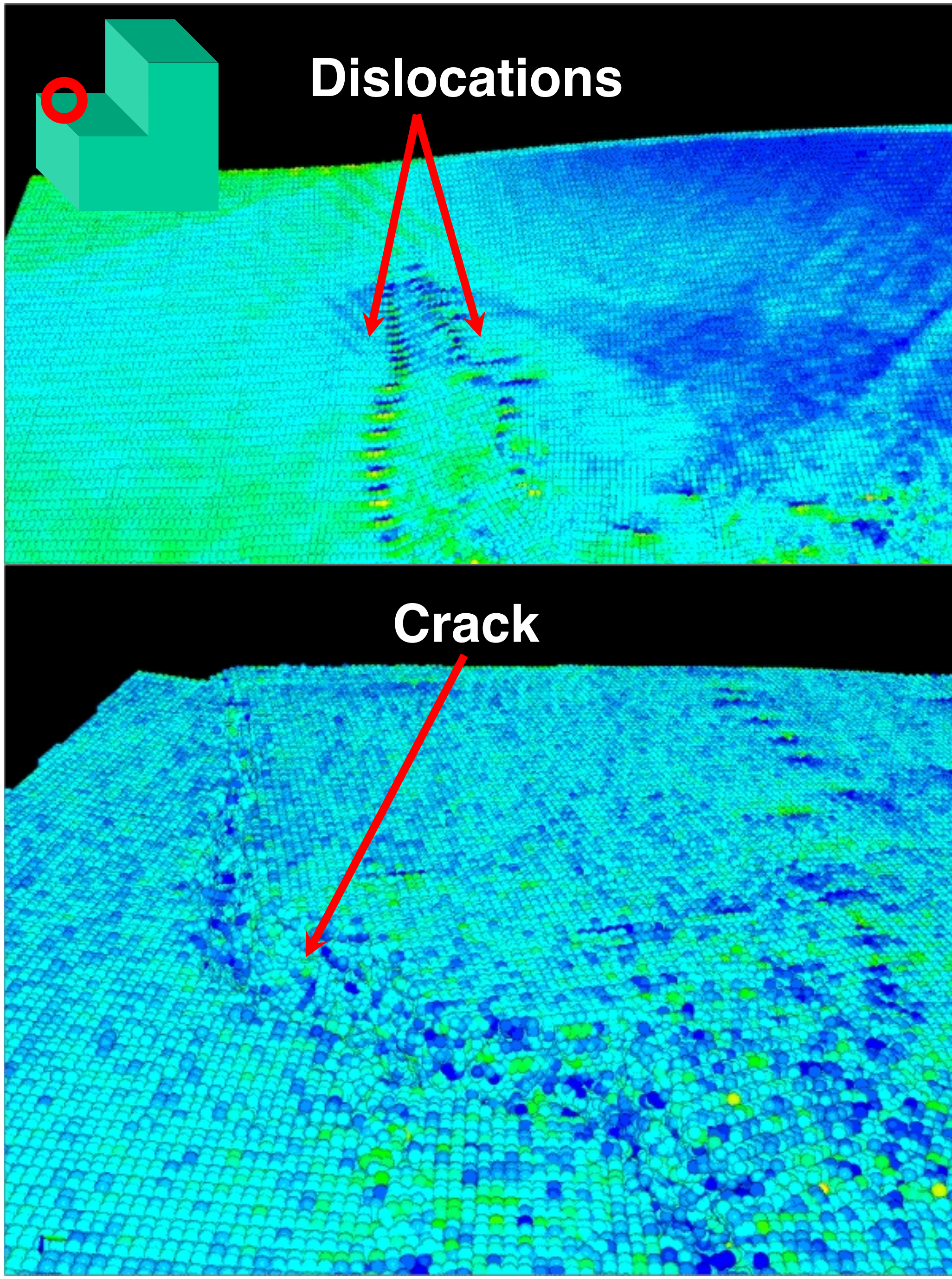


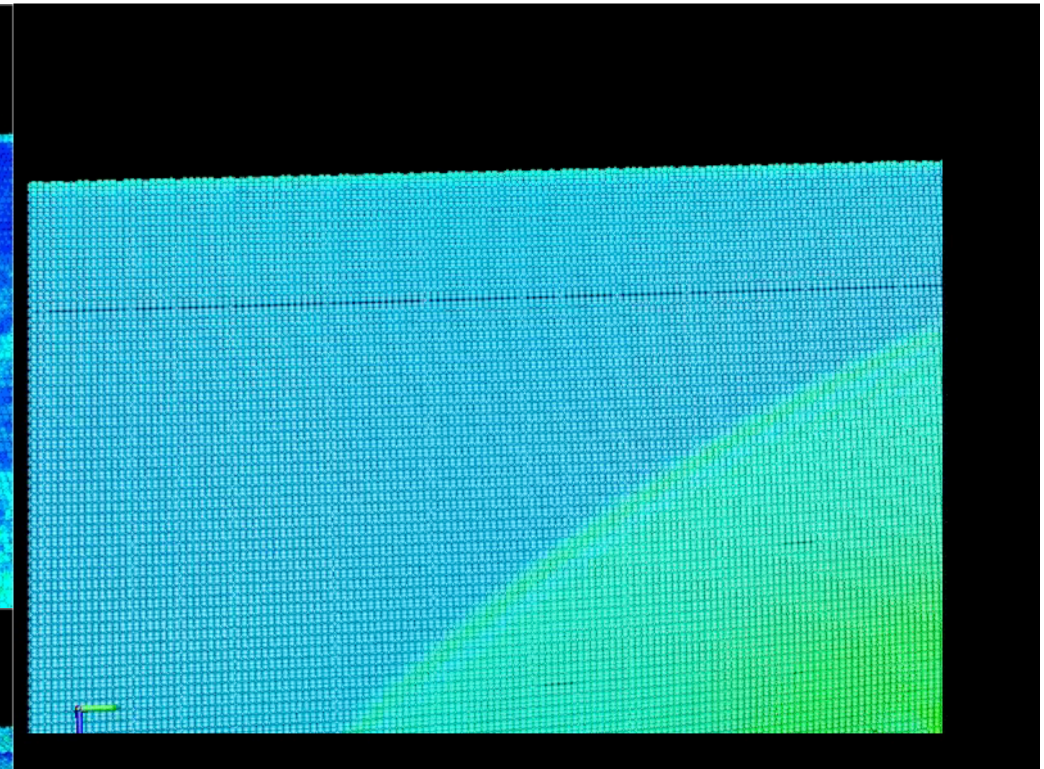




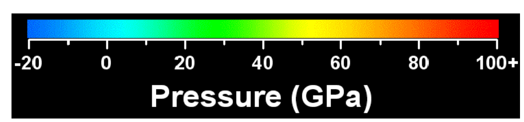
209 million atom MD of hypervelocity impact in AlN for the design of light-weight ceramic armors

Crack Nucleation at Kink Bands



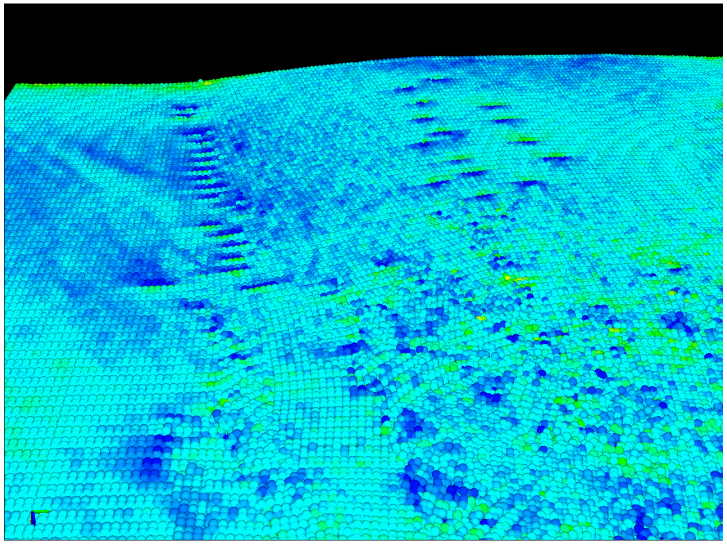


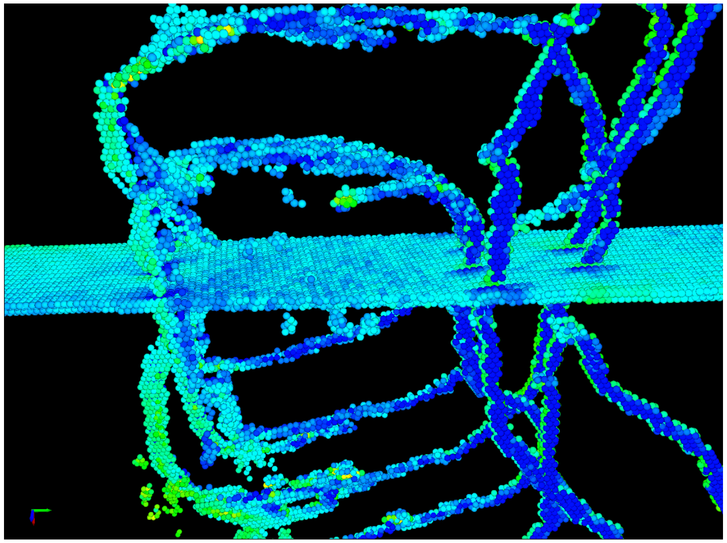
- Series of dislocation dipoles with opposite Burgers vectors form a kink band to releases stress
- Tilt grain boundaries of the kink bands act as sources of mode-II (shear) crack nucleation



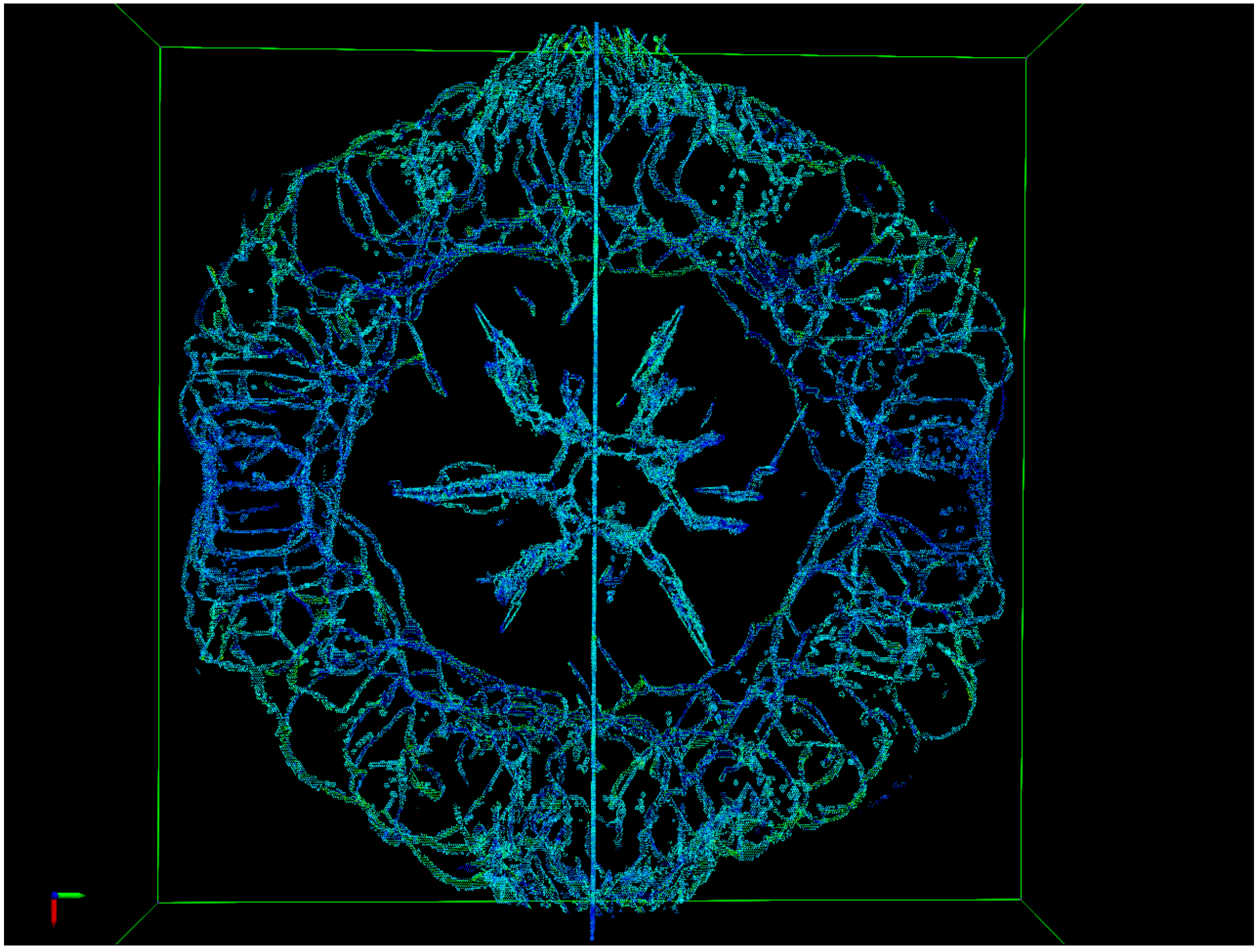
Dislocation Loops at Kink Bands

Graph (shortest-path circuit) based mining of topological defects





Atoms participating in non-6-member circuits



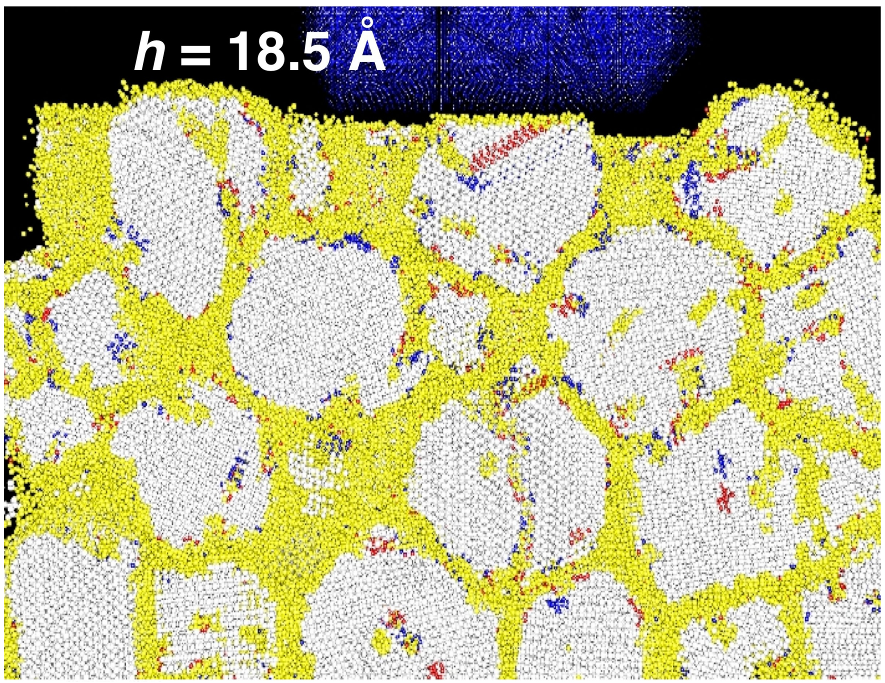
Dislocation network

Nanoindentation on Nanophase SiC

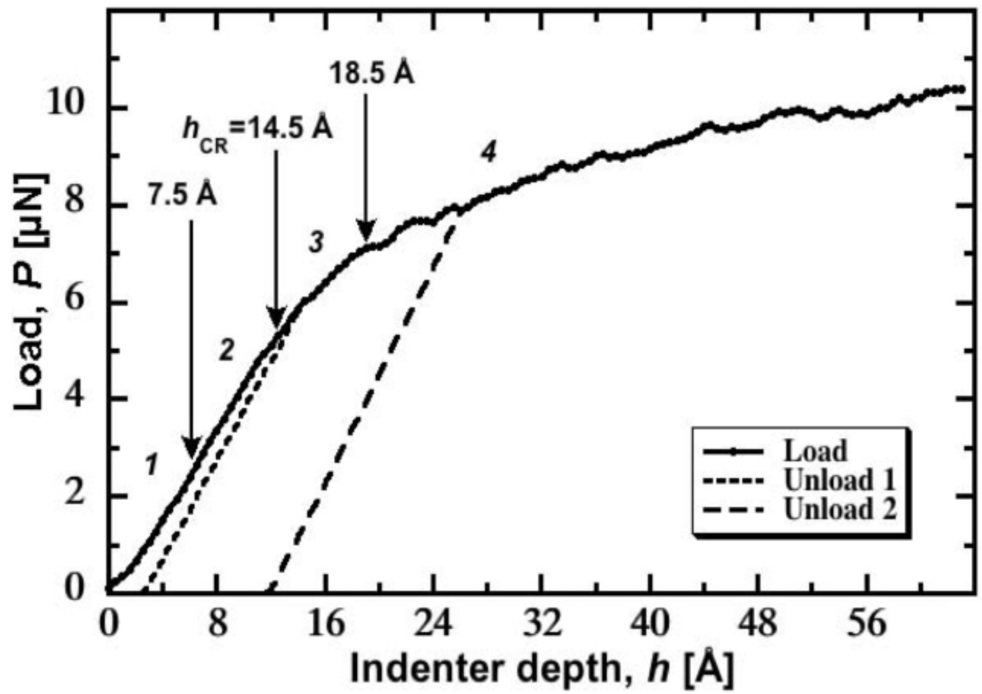
Superhardness

MD: 39 GPa
(grain size, *d* = 8 nm)

Expt.: 30-50 GPa
(*d* = 5-20 nm)
[Liao *et al*., *APL*, '05]



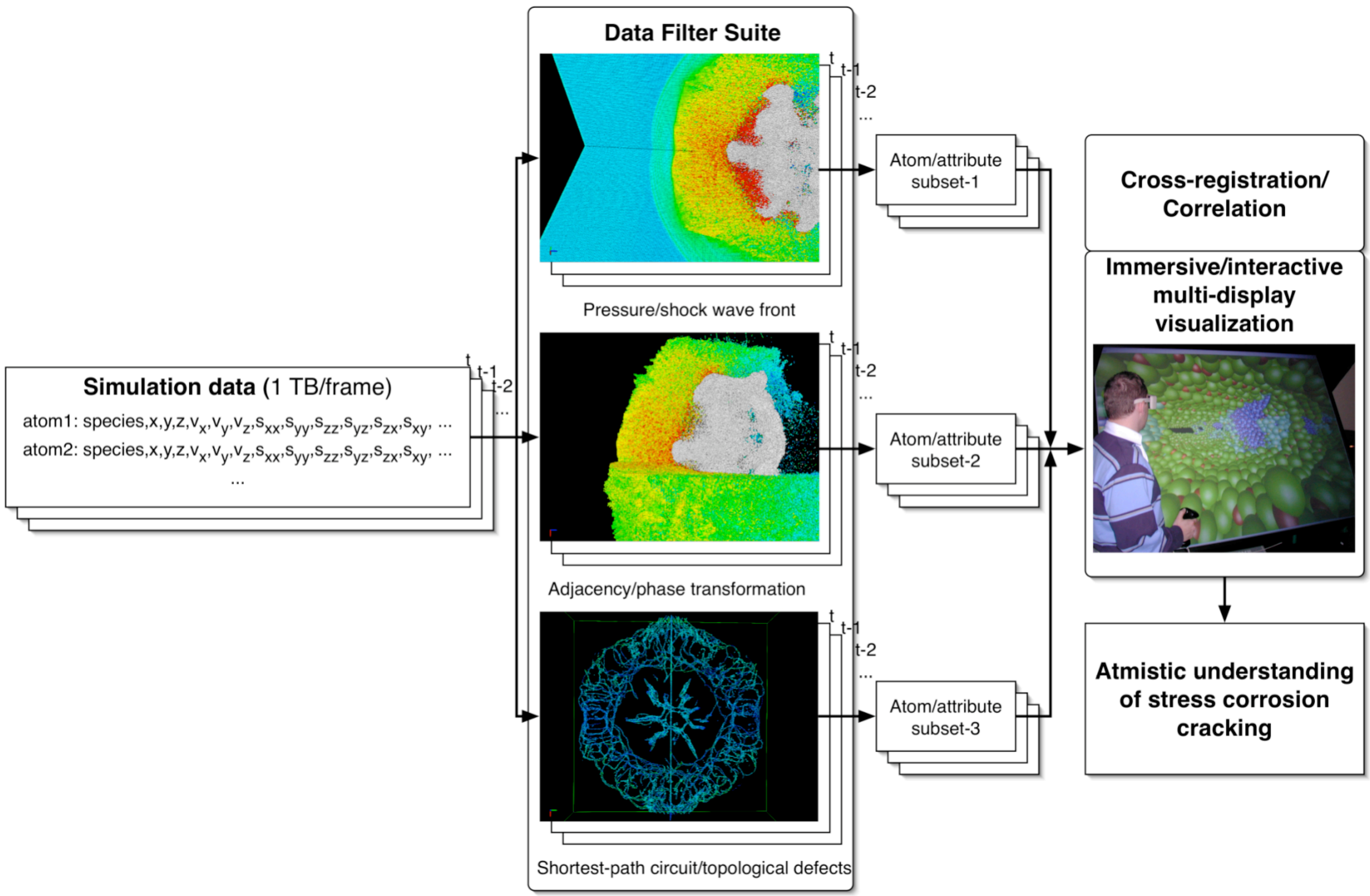
Load-displacement curve



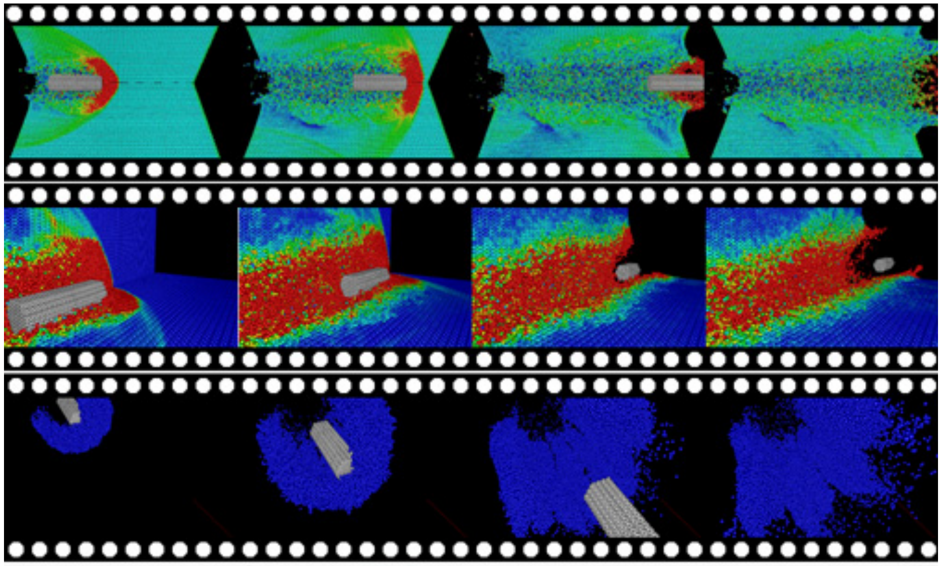
Crossover from intergrain continuous response to intragranular discrete response

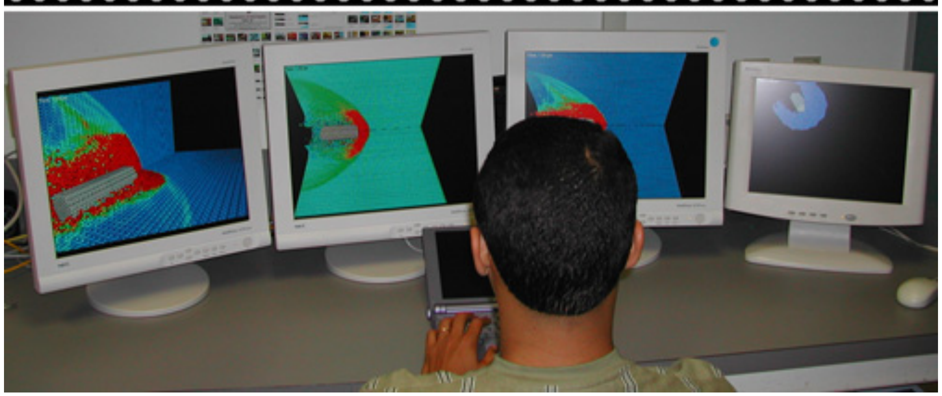
Szlufarska, Nakano & Vashishta, *Science* **309**, 911 ('05)

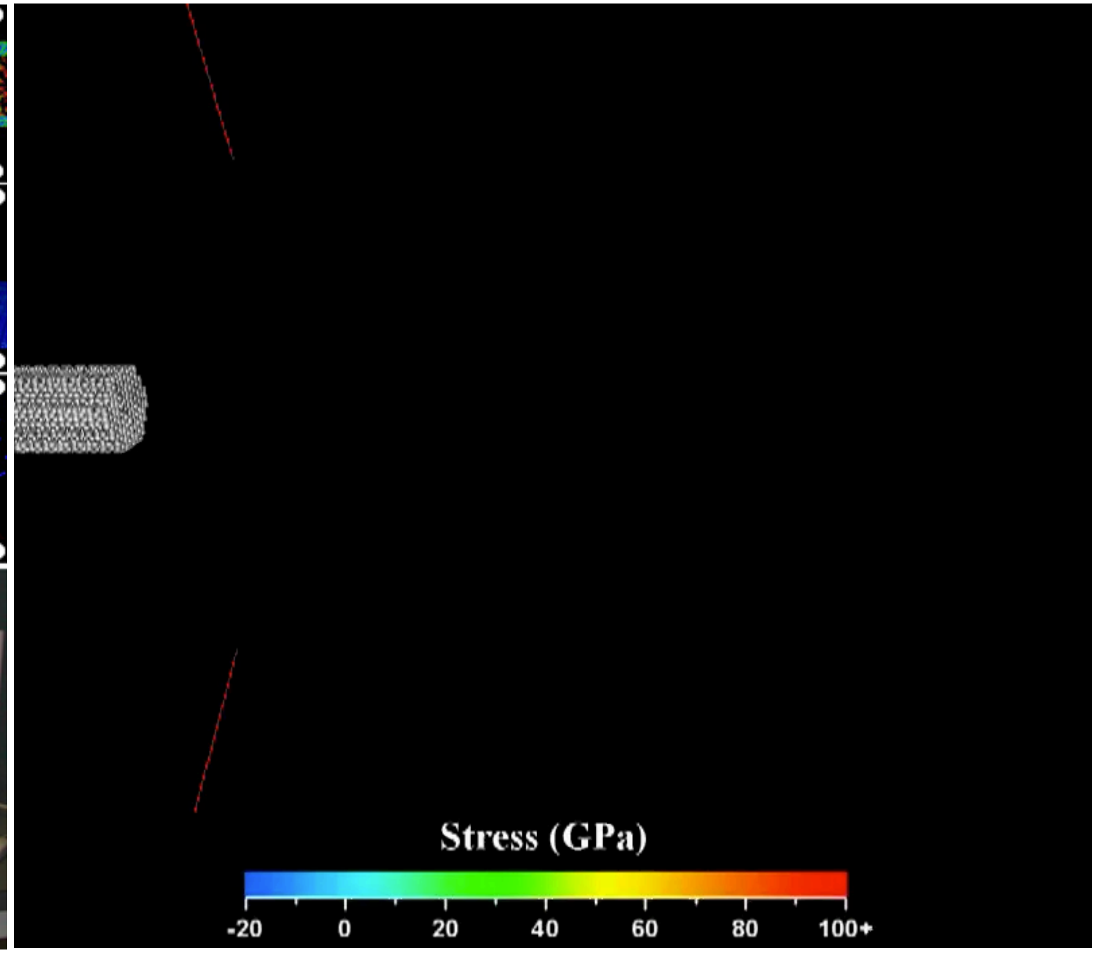
Data Mining on a Grid

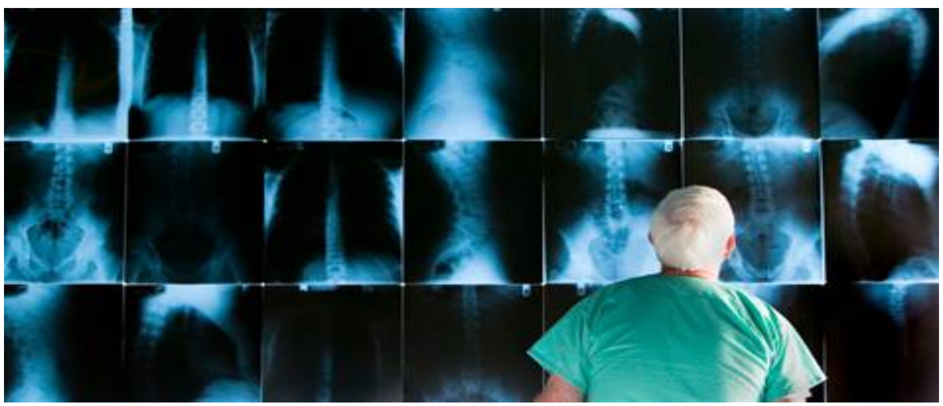


Multimodal Multidisplay Visualization









Hypervelocity penetration through an AlN plate

Singular Value Decomposition & Data Mining

Aiichiro Nakano

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Data mining $\cong$ data compression

Rank of a Matrix

- ***N*×*M* matrix *A* as a mapping: $R^M \rightarrow R^N$**

$$
\begin{array}{cc} & 1 \\ M & \begin{bmatrix} \\ x \\ \\ \end{bmatrix} \end{array}
\quad x\left(\in R^M\right) \xrightarrow[A]{} b = Ax\left(\in R^N\right) \quad
\begin{array}{cc} 1 & \\ \begin{bmatrix} \\ b \\ \\ \\ \end{bmatrix} & N \end{array}
$$

- **Range of *A*: Vector space $\{b = Ax | \forall x\}$**
- **Rank of *A*: Number of linearly-independent vectors in the range, *i.e.*, how many linearly-independent *N*-element vectors are there in the range, such that**

$$b = A^{\forall}x = \sum_{\nu=1}^{m} c_\nu \left|\nu\right\rangle$$

Low Rank Approximations of a Matrix

- **Rank-1 approximation: $NM \rightarrow N + M$**

$$\begin{array}{cc} & \boldsymbol{M} \\ \boldsymbol{N} & \begin{bmatrix} \quad & & \quad \\ & \psi & \\ & & \end{bmatrix} \end{array} \cong \begin{bmatrix} \\ u \\ \\ \end{bmatrix} \begin{bmatrix} \quad & v & \quad \end{bmatrix}$$

- **Rank-2 approximation: $NM \rightarrow 2(N + M)$**

$$\begin{bmatrix} \quad & & \quad \\ & \psi & \\ & & \end{bmatrix} \cong \begin{bmatrix} \\ u_1 \\ \\ \end{bmatrix} w_1 \begin{bmatrix} \quad & v_1 & \quad \end{bmatrix} + \begin{bmatrix} \\ u_2 \\ \\ \end{bmatrix} w_2 \begin{bmatrix} \quad & v_2 & \quad \end{bmatrix}$$

- **Rank-m ($m << N, M$) approximation: $NM \rightarrow m(N + M)$**

$$\begin{bmatrix} \quad & & \quad \\ & \psi & \\ & & \end{bmatrix} \cong \sum_{\nu=1}^{m} \begin{bmatrix} \\ u_\nu \\ \\ \end{bmatrix} w_\nu \begin{bmatrix} \quad & v_\nu & \quad \end{bmatrix}$$

Singular Value Decomposition

- **Problem:** Optimal approximation of an $N \times M$ matrix ψ of rank-m ($m \ll N$)?
- **Theorem:** An $N \times M$ matrix ψ (assume $N \geq M$) can be decomposed as

$$\psi = UDV^T = \sum_{\nu=1}^{M} U_{i\nu} d_\nu V_{j\nu} = \sum_{\nu=1}^{M} u_i^{(\nu)} d_\nu v_j^{(\nu)}$$

where $U \in R^N \times R^M$ & $V \in R^M \times R^M$ are column orthogonal & D is diagonal

$$U^T U = V^T V = I_M$$

$$\begin{array}{cc} & M \\ N & \begin{bmatrix} & & \\ & \psi & \\ & & \end{bmatrix} \end{array} = \underbrace{\begin{bmatrix} & & \\ & U & \\ & & \end{bmatrix}}_{N \times M} \underbrace{\begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_M \end{bmatrix}}_{M \times M} \underbrace{\begin{bmatrix} & & \\ & V^T & \\ & & \end{bmatrix}}_{M \times M}$$

- **Theorem:** Sort the SVD diagonal elements in descending order $d_1 \geq d_2 \geq \ldots$ & retain the first m terms

$$\psi^{(m)} \equiv \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T}$$

which is optimal among $\forall$rank-m matrices in the 2-norm sense with the error

$$\min_{rank(A)=m} \|A - \psi\|_2 = \left\|\psi^{(m)} - \psi\right\|_2 = d_{m+1}$$

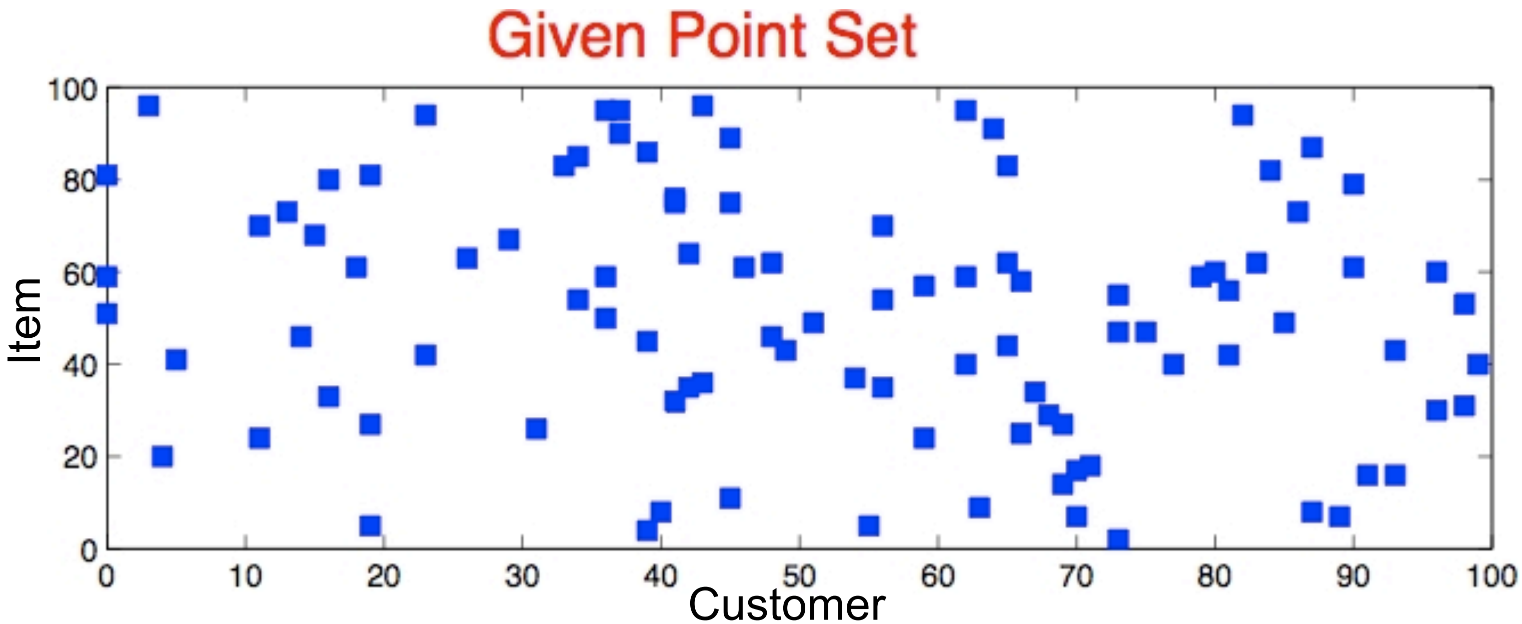
SVD for Image Compression

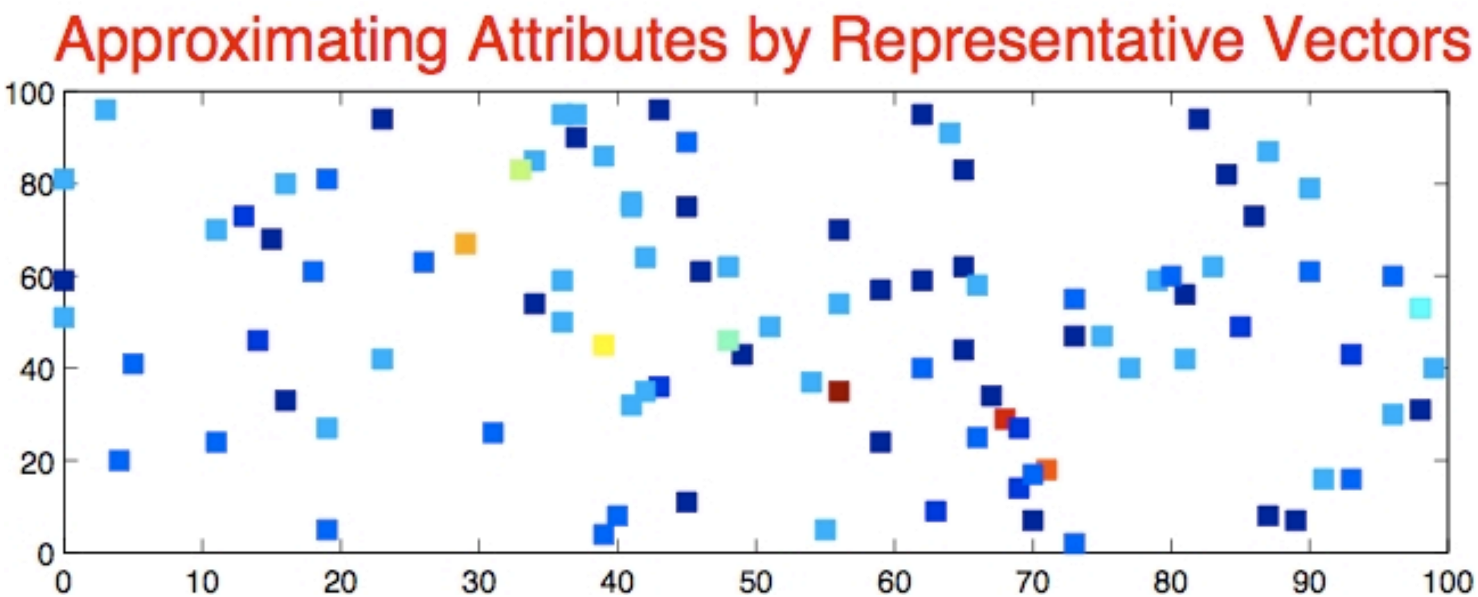
Original Image | 5 Iterations | 10 Iterations

20 Iterations | 60 Iterations | 100 Iterations

D. Richards & A. Abrahamsen

SVD in Data Mining





N. Ramakrishnan & A. Y. Grama

Machine Learning in Simulation

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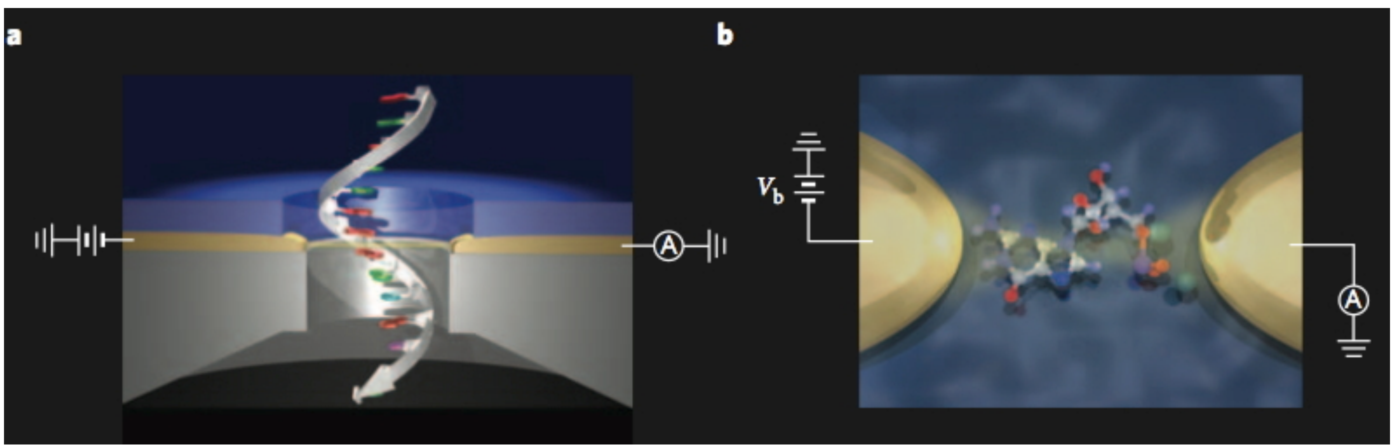
Rapid Genome Sequencing

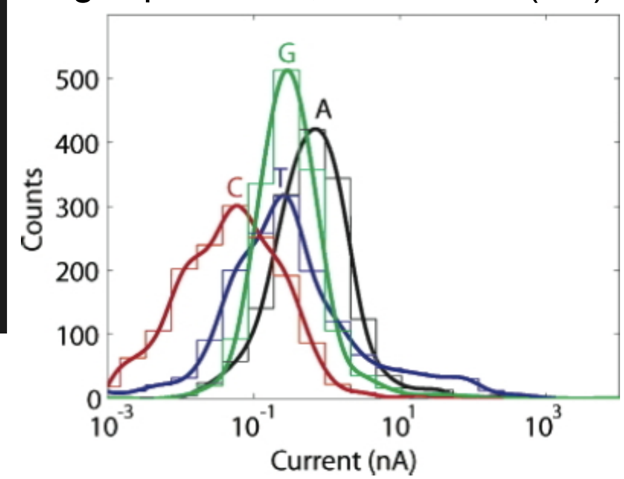
- **$10M Archon X prize for decoding 100 human genomes in 10 days & < $10K per genome (**http://genomics.xprize.org**): Preemptive attack on diseases**

- **Quantum tunneling current for rapid DNA sequencing?**



Tsutsui *et al.*, *Nature Nanotechnology* **5**, 286 ('10);
Girdhar *et al.*, *PNAS* **110**, 16748 ('13)

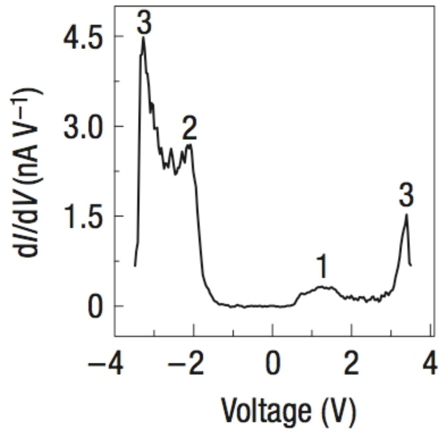
Lagerqvist *et al.*, *Nano Lett.* ('06)



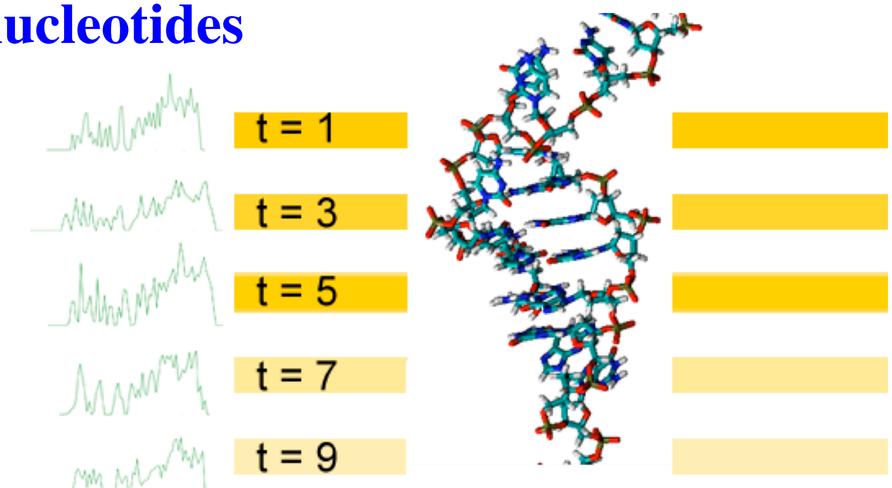
- **Tunneling current alone cannot distinguish the 4 nucleotides (A, C, G, T)**

Rapid DNA Sequencing *via* Machine Learning

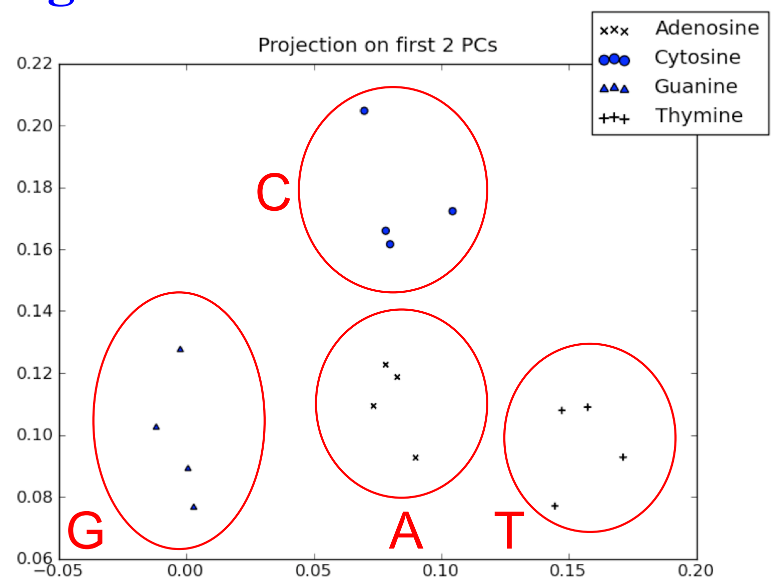
- **Use tunneling current (I)-voltage (V) characteristic (or electronic density-of-states) as the 'fingerprints' of the 4 nucleotides**

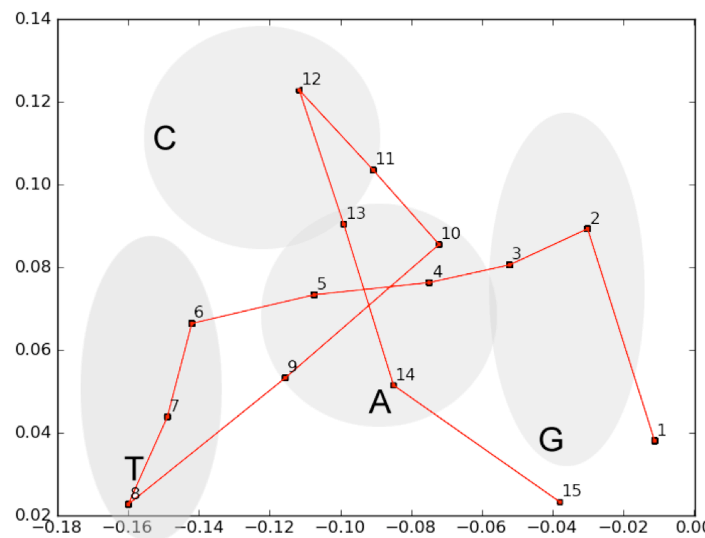


Shapir *et al.*,
Nature Materials ('08)



- **Principal component analysis (PCA) & fuzzy c-means clustering clearly distinguish the 4 nucleotides**





- **Viterbi algorithm for even higher-accuracy sequencing** Yuen *et al*, *IJCS* **4**, 352 ('10)

Post-Exaflop/s: AI for Science

- A series of townhall meetings by U.S. Department of Energy (DOE) to plan post-exascale science

DOE readies multibillion-dollar AI push

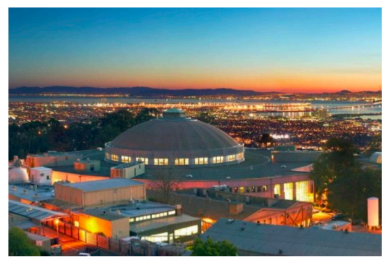
U.S. supercomputing leader is the latest big backer in a globally crowded field

By **Robert F. Service**, *in Washington, D.C.*

Science **366**, 559 (Nov. 1, '19)

Chicago AI for Science Town Hall
Argonne National Laboratory
July 22-23, 2019
Registration for Chicago: CLOSED
Town Hall Agenda: Click here
Questions for Chicago?
Contact: smulligan@anl.gov

Oak Ridge AI for Science Town Hall
Oak Ridge National Laboratory
August 20-21, 2019
To register for Oak Ridge, click here
DRAFT Agenda: Click here
Questions for Oak Ridge?
Contact: verasteguirj@ornl.gov

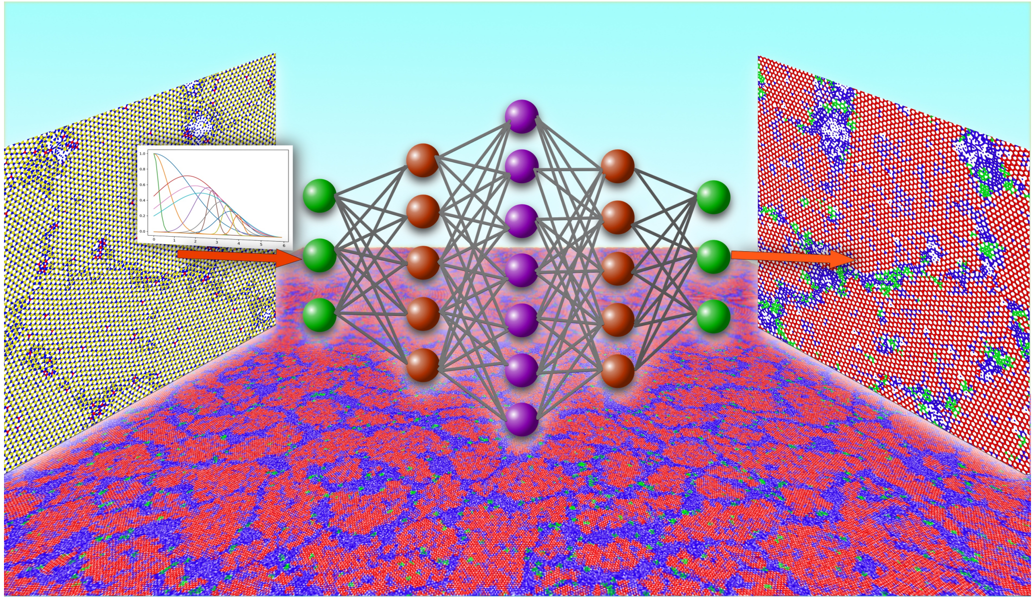


Berkeley AI for Science Town Hall
Lawrence Berkeley National Laboratory
September 11-12, 2019
To register for Berkeley, click here
DRAFT Agenda: Click here
Questions for Berkeley?
Contact: latheobald@lbl.gov

Washington DC AI for Science Town Hall
October 22-23, 2019
To register for DC, click here
DRAFT Agenda: Click here
Questions for DC?
Contact: DC-AI-TownHall@ornl.gov

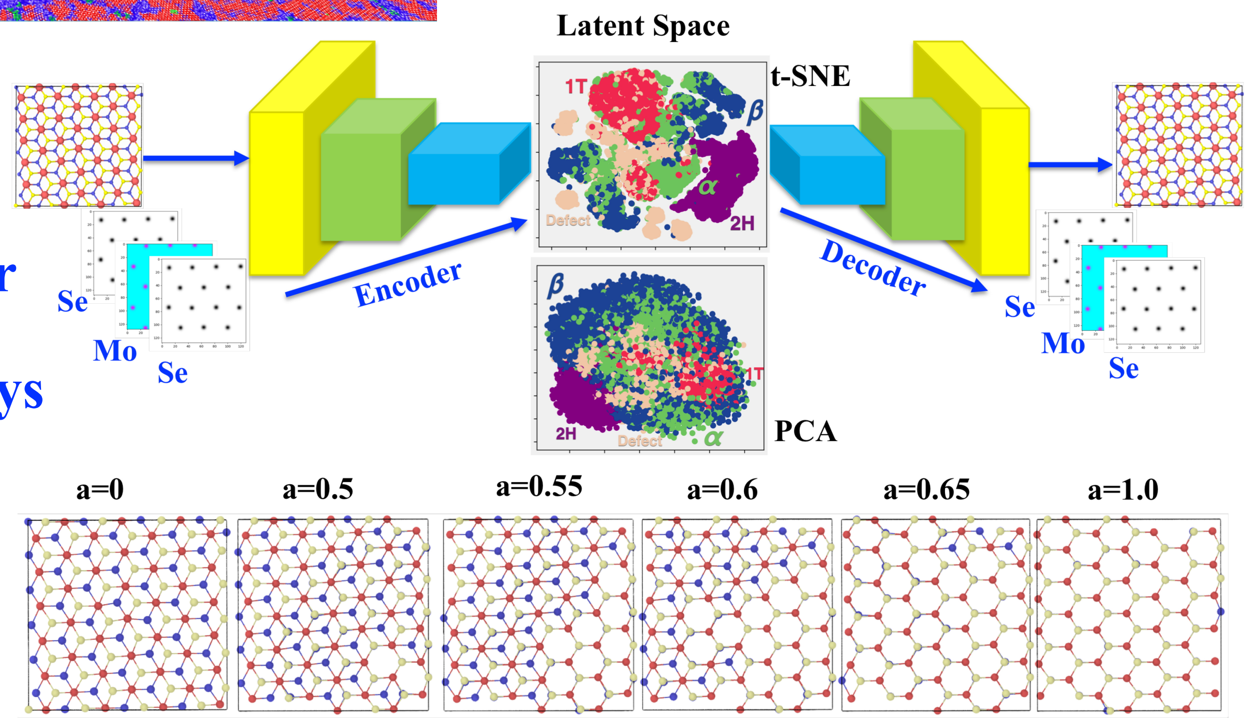
- AI for science: Convergence of high performance computing (HPC) & artificial intelligence (AI) to integrate simulation, experiment, data & learning

Learning Materials Phases & Defects



- **Feedforward neural network to learn phases from local symmetry functions**

K. Liu *et al.*, *Proc. ScalA18* ('18)
S. Hong *et al.*, *JPCL* **10**, 2739 ('19)

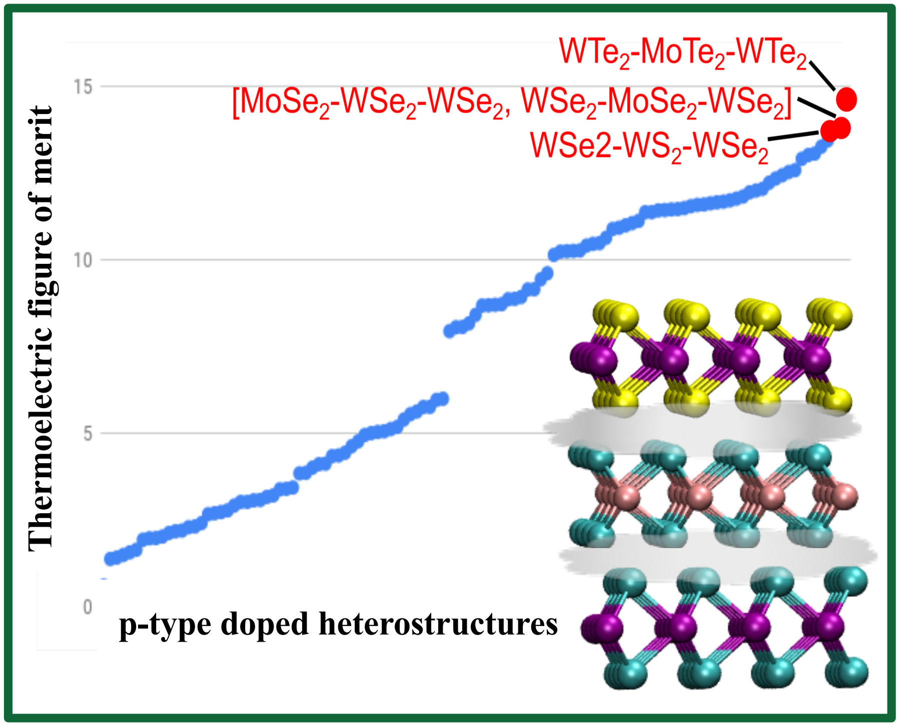


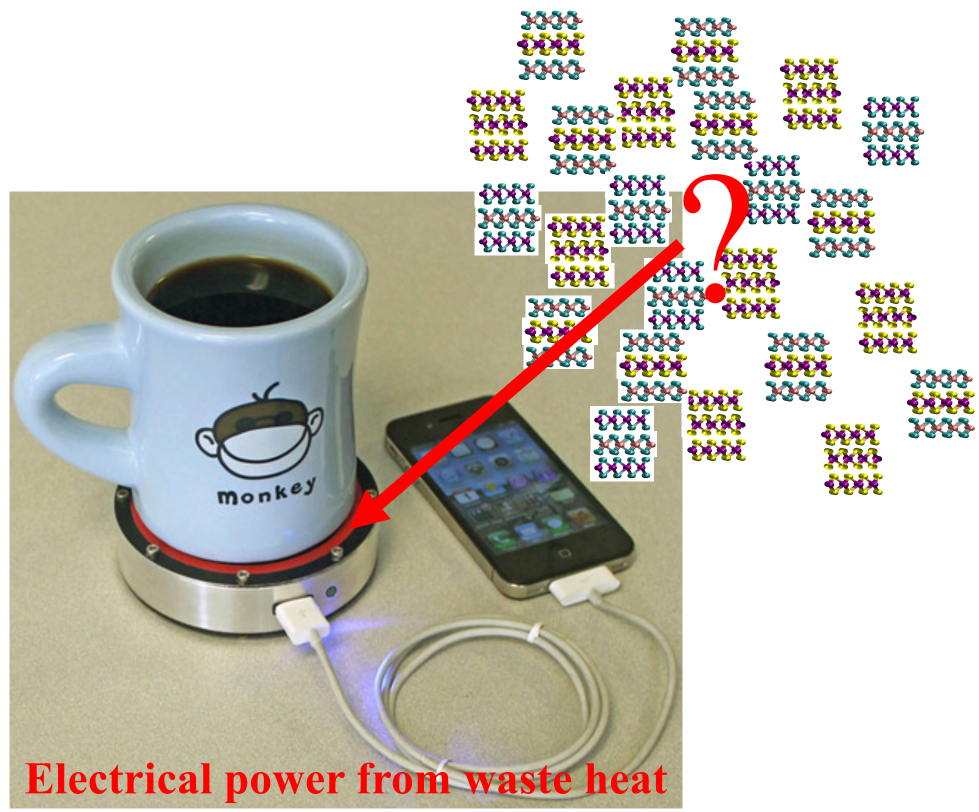
- **Variational autoencoder to generate transformation pathways from images & latent-space algebra**

P. Rajak *et al.*, *Phys. Rev. B* **100**, 014108 ('19)

Active Learning of Optimal Materials

- **Bayesian optimization balances exploitation & exploration to find a structure with the desired property with a minimal number of quantum-mechanical calculations**
- **Predicted three-layered transition-metal chalcogenide (TMDC) heterostacks with the largest thermoelectric figure-of-merit**

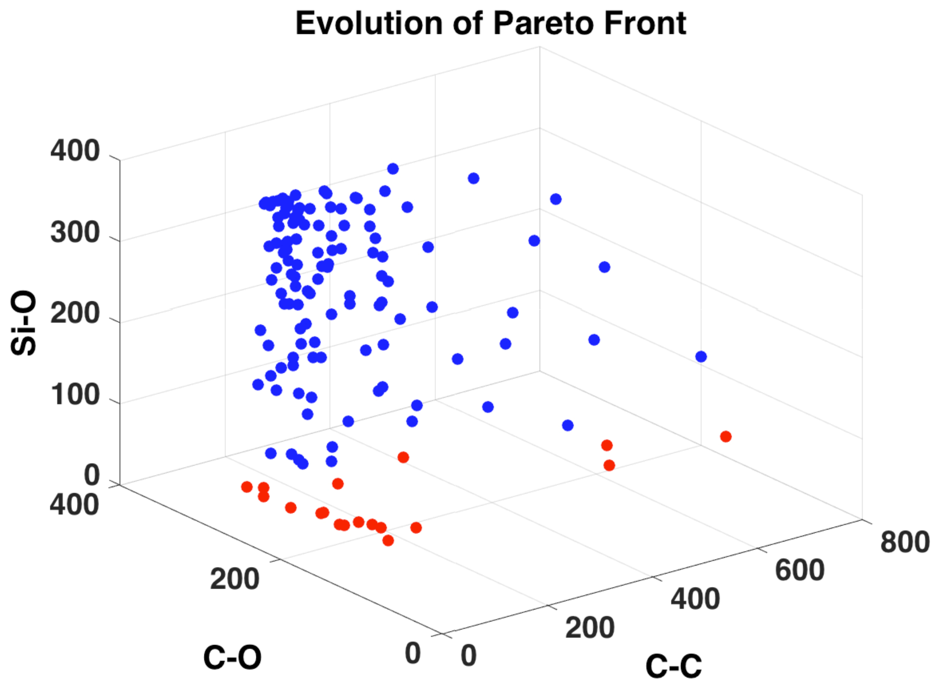


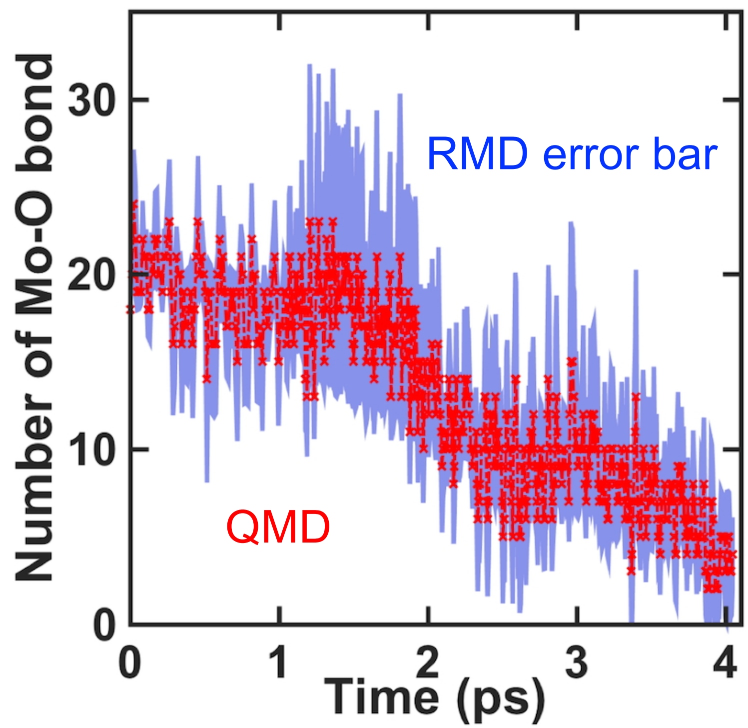


L. Bassman *et al*., *npj Comput. Mater.* **4**, 74 ('18)

Pareto-Frontal Uncertainty Quantification

- **Train reactive force-field parameters by dynamically fitting reactive molecular dynamics (RMD) trajectories to quantum molecular dynamics (QMD) trajectories on-the-fly**
- **Pareto optimal front in multiobjective genetic algorithm (MOGA) provides an ensemble of force fields to enable uncertainty quantification (UQ)**





- Pareto-optimal solutions during genetic training (RMD errors for three quantities-of-interest)
- Converged Pareto-optimal front

A. Mishra *et al.*, *npj Comput. Mater.* **4**, 42 ('18)