

# Hybrid Particle-Continuum Simulation

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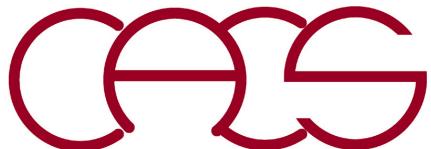
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*Department of Chemical Engineering & Materials Science*  
*Department of Biological Sciences*

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Adaptively manage accuracy-cost  
trade-off; coarse-graining by heuristics  
(*i.e.*, switching to different abstract)



# Multiscale Modeling

## The Nobel Prize in Chemistry 2013



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Martin Karplus



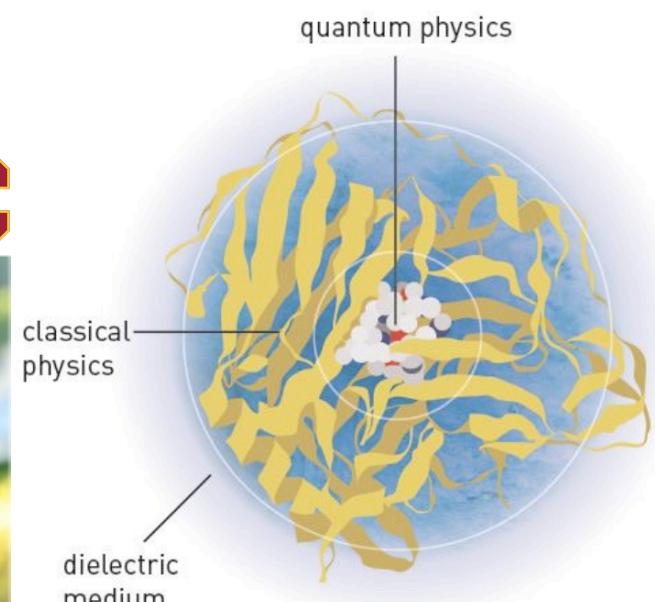
Photo: Keilana via  
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Michael Levitt



Photo: Wikimedia  
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Arieh Warshel

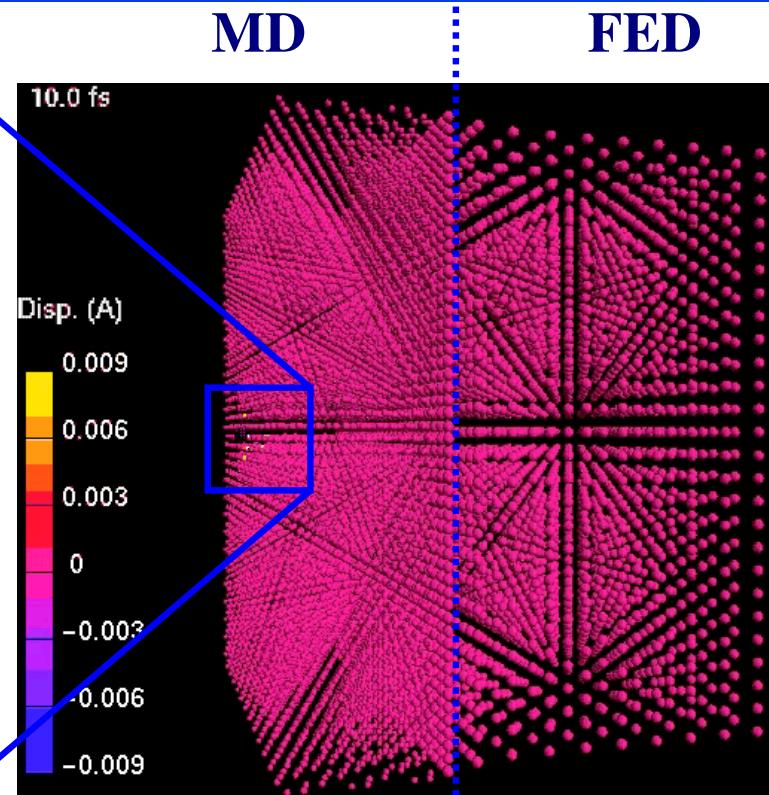
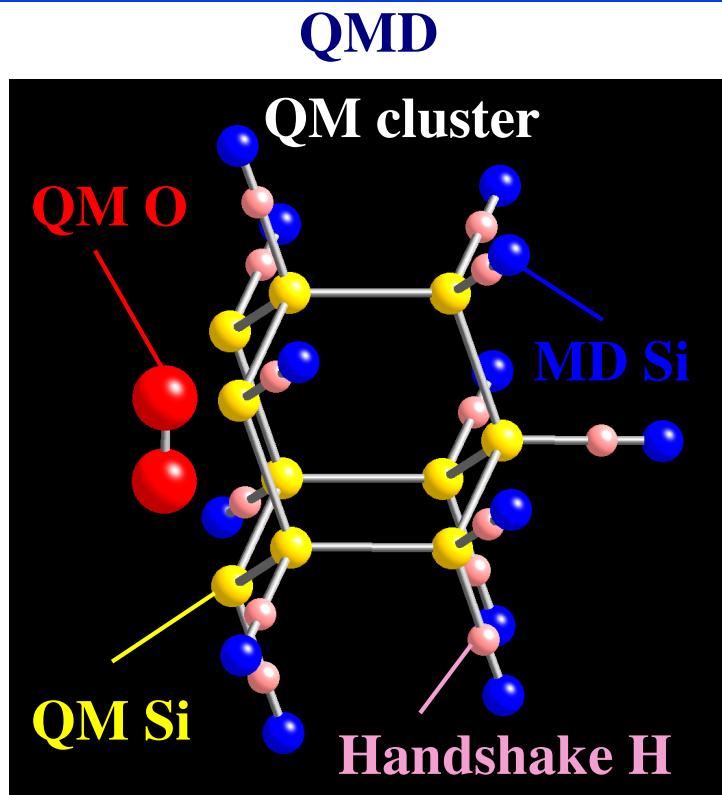


**QM/MM:**  
**quantum-**  
**mechanical/molecular-**  
**mechanical modeling**

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*. A. Warshel & M. Karplus, *J. Am. Chem. Soc.* **94**, 5612 ('72)  
A. Warshel & M. Levitt, *J. Mol. Biol.* **103**, 227 ('76)

**Find multiscale modeling in your area!**

# Adaptive Multiscale Dynamics



## Oxidation of Si

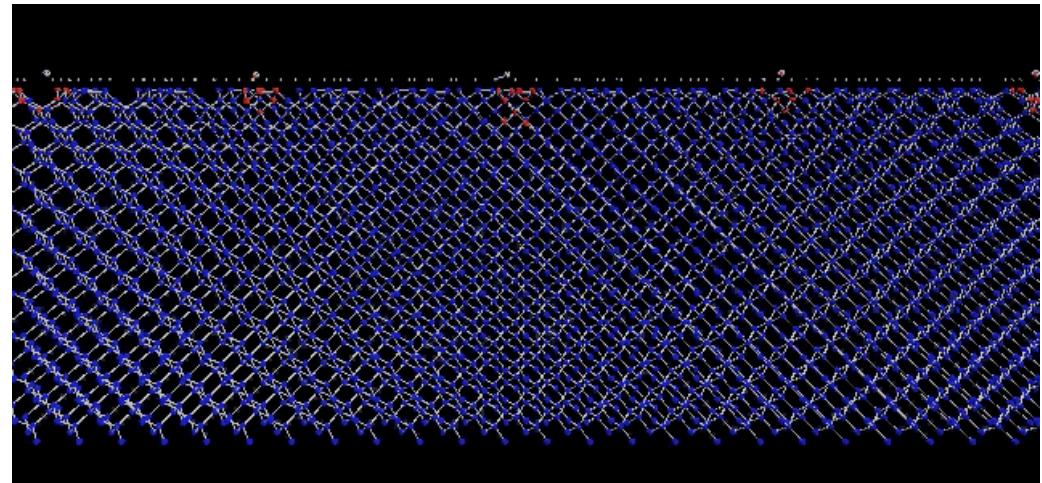
S. Ogata *et al.*, *Comput. Phys. Commun.* **138**, 143 ('01)

L. Lidorikis *et al.*, *Phys. Rev. Lett.* **87**, 086104 ('01)

**QMD/MD/FED:**  
quantum molecular dynamics/  
molecular dynamics/  
finite-element dynamics simulation

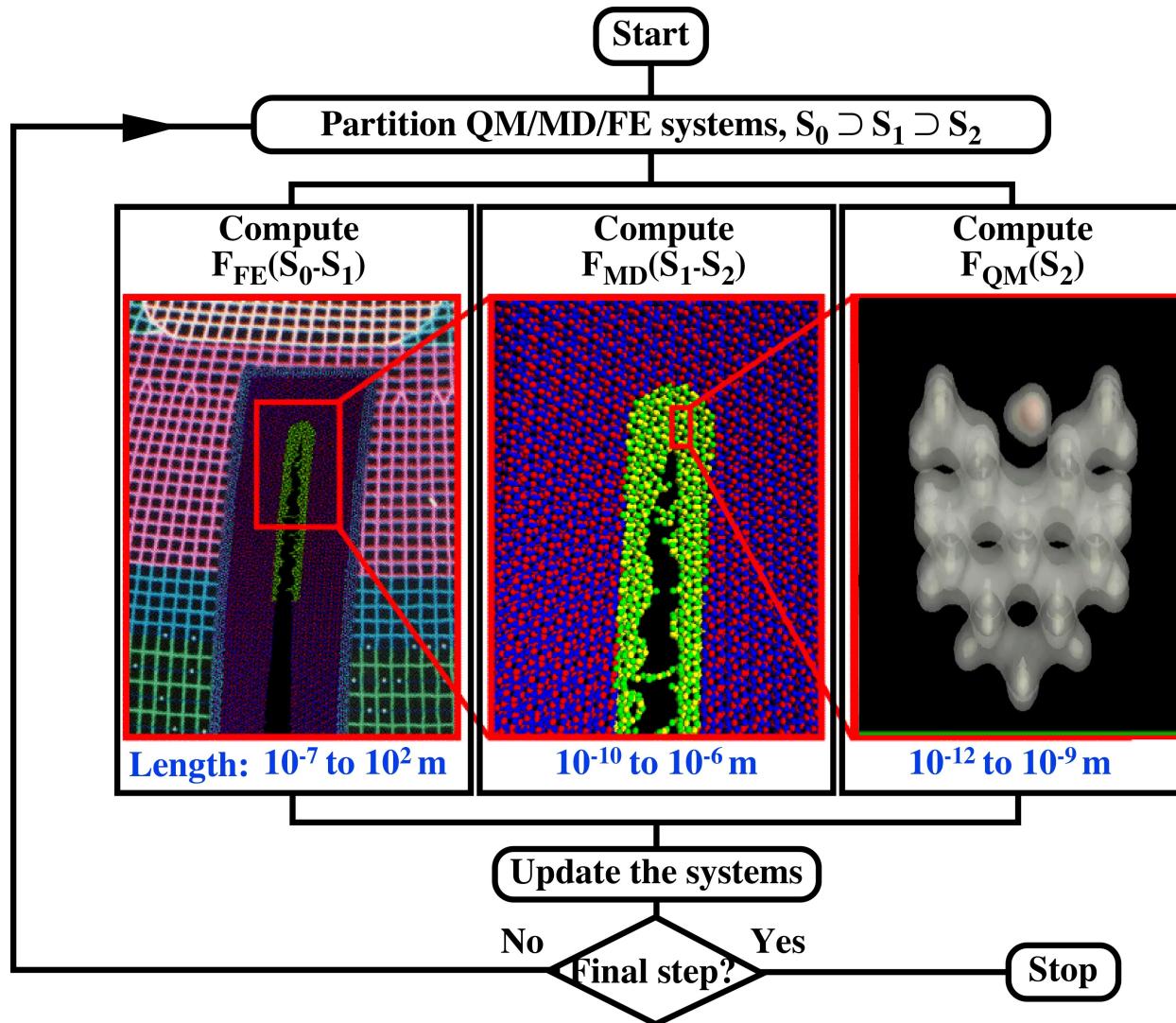
High-energy  
beam oxidation  
of Si (SIMOX)

H. Takemiya *et al.*,  
*IEEE/ACM Supercomputing (SC06)*



# Multiscale FED/MD/QMD Simulation

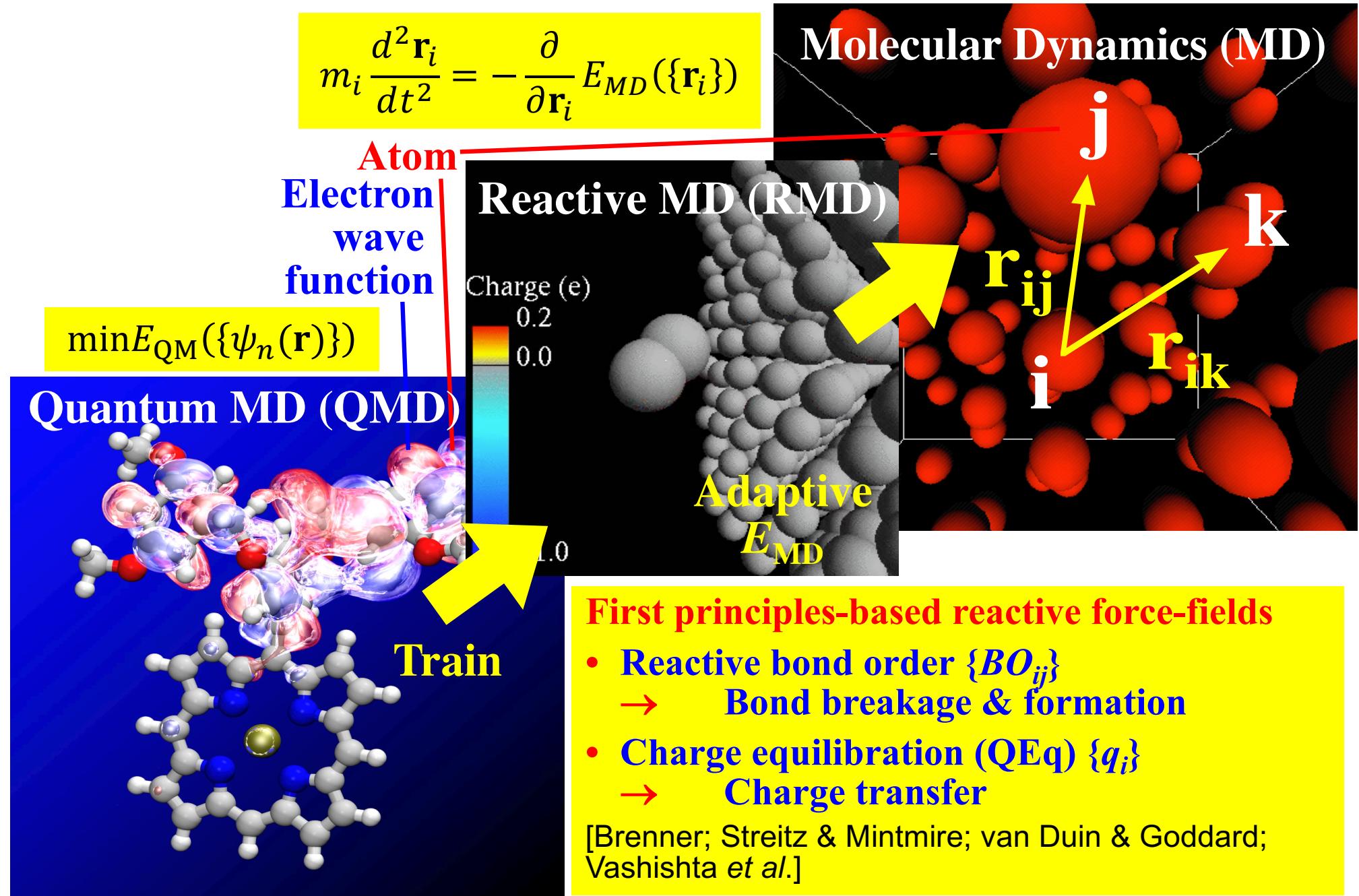
- Embed high-accuracy computations only when & where needed
- Train coarse simulations by fine simulations



**Multiscale simulation to seamlessly couple:**

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

# Hierarchical Atomistic Simulation Methods



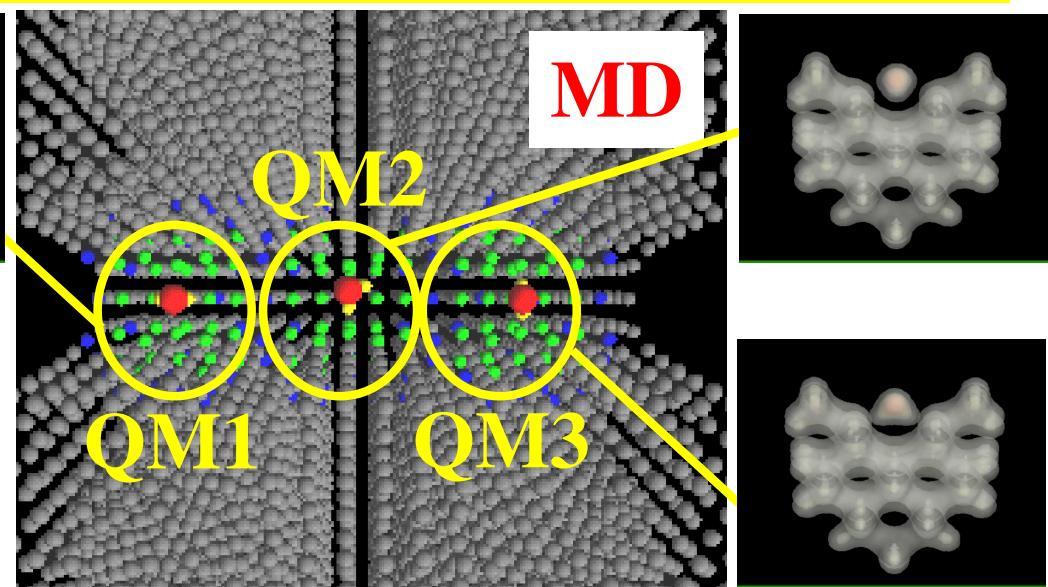
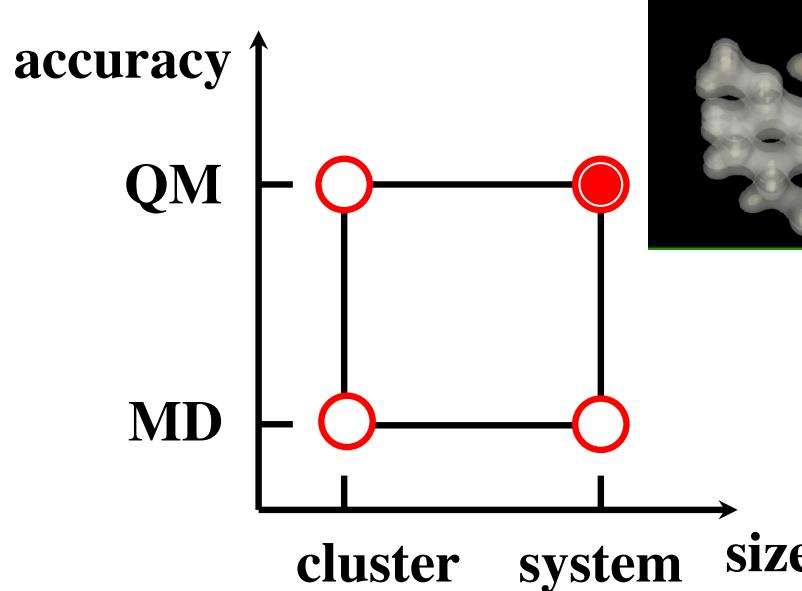
# DC Multiscale MD/QM (DFT)

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

- Extrapolation in meta-model space (accuracy vs. size)
- Modular
  - Reuse of existing MD & QM (density functional theory) codes
  - Minimal inter-model dependence/communication

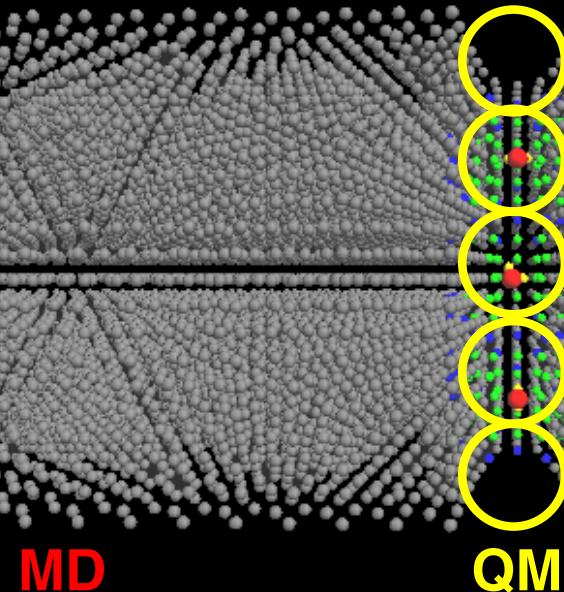
## Divide-&-conquer DFT embedded in MD

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



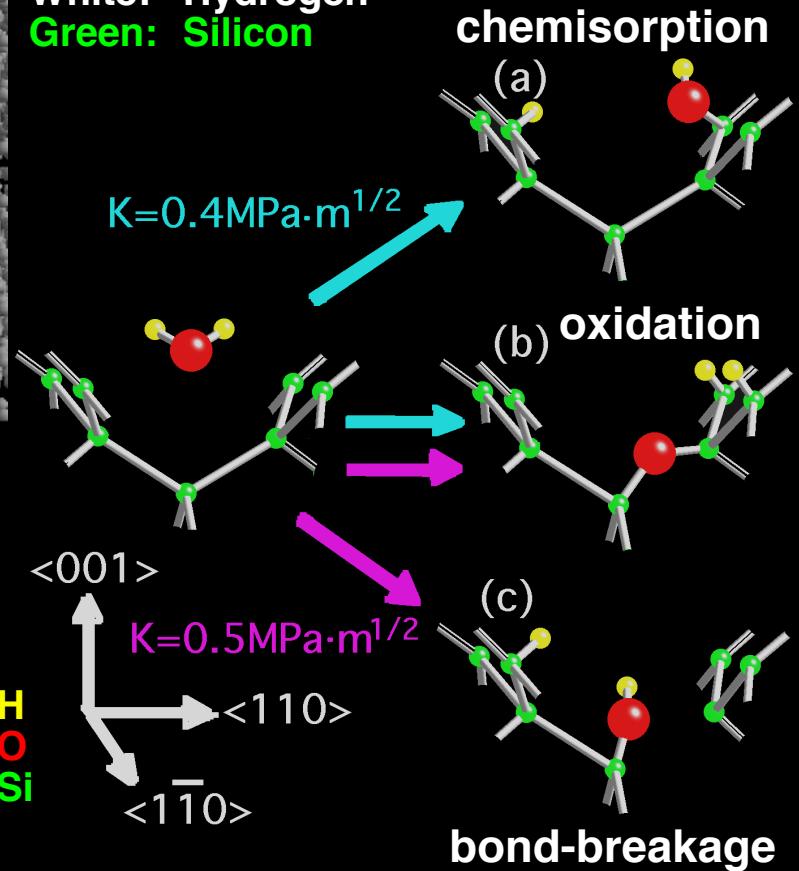
# Environmental Effect on Fracture

## Reaction of H<sub>2</sub>O molecules at a Si crack tip



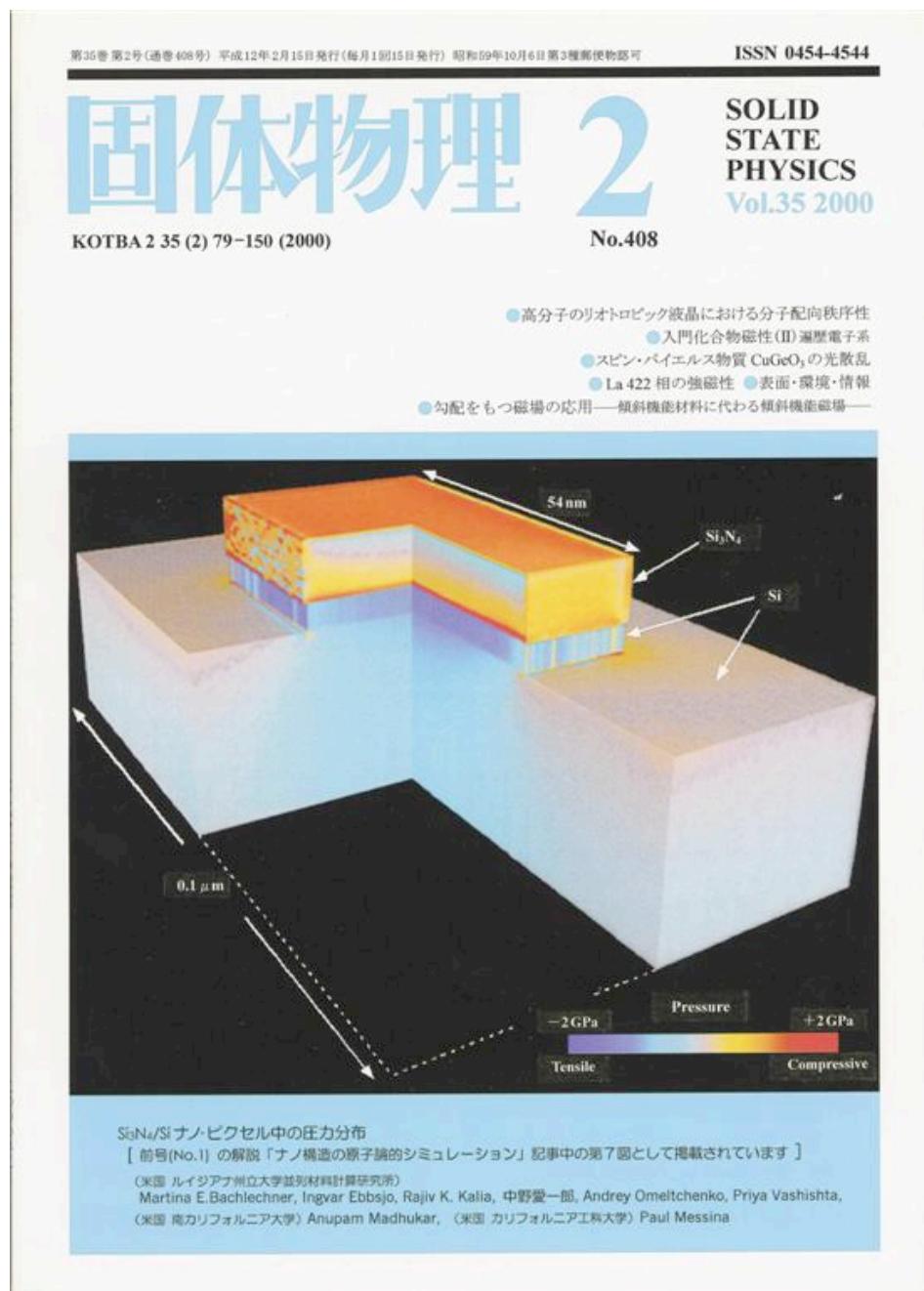
Collaborators: S. Ogata (NIT),  
F. Shimojo (Kumamoto)

Blue: Oxygen  
White: Hydrogen  
Green: Silicon



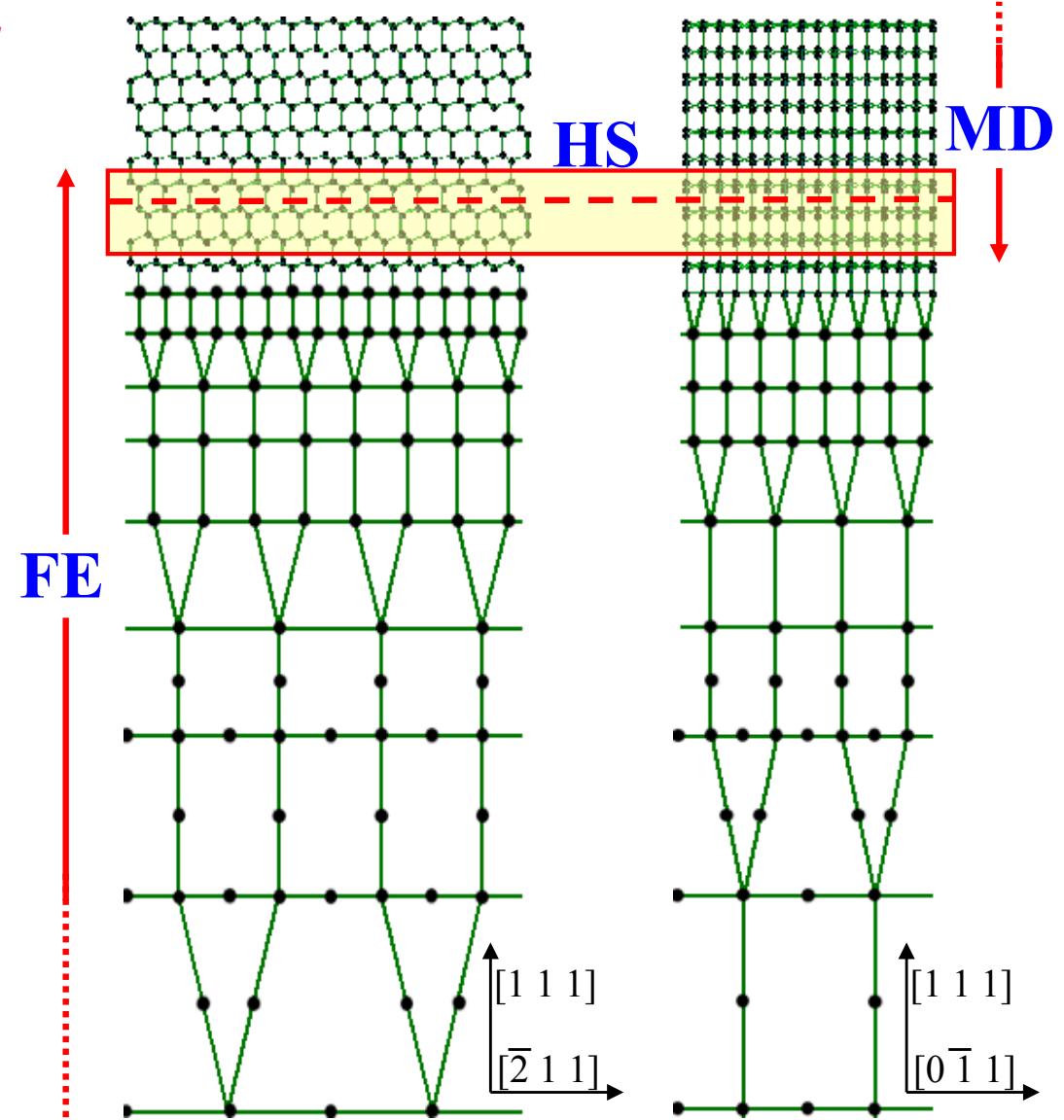
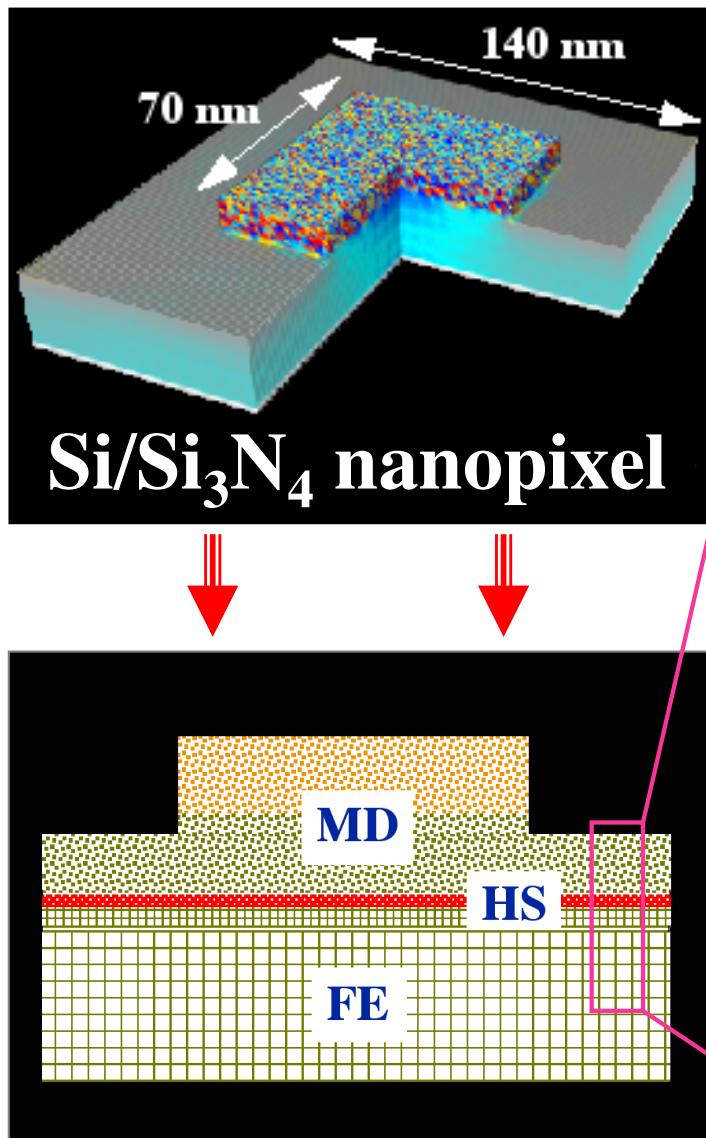
Significant dependence of the  
reaction on stress intensity factor

# Atomistic Simulations of Nanodevices



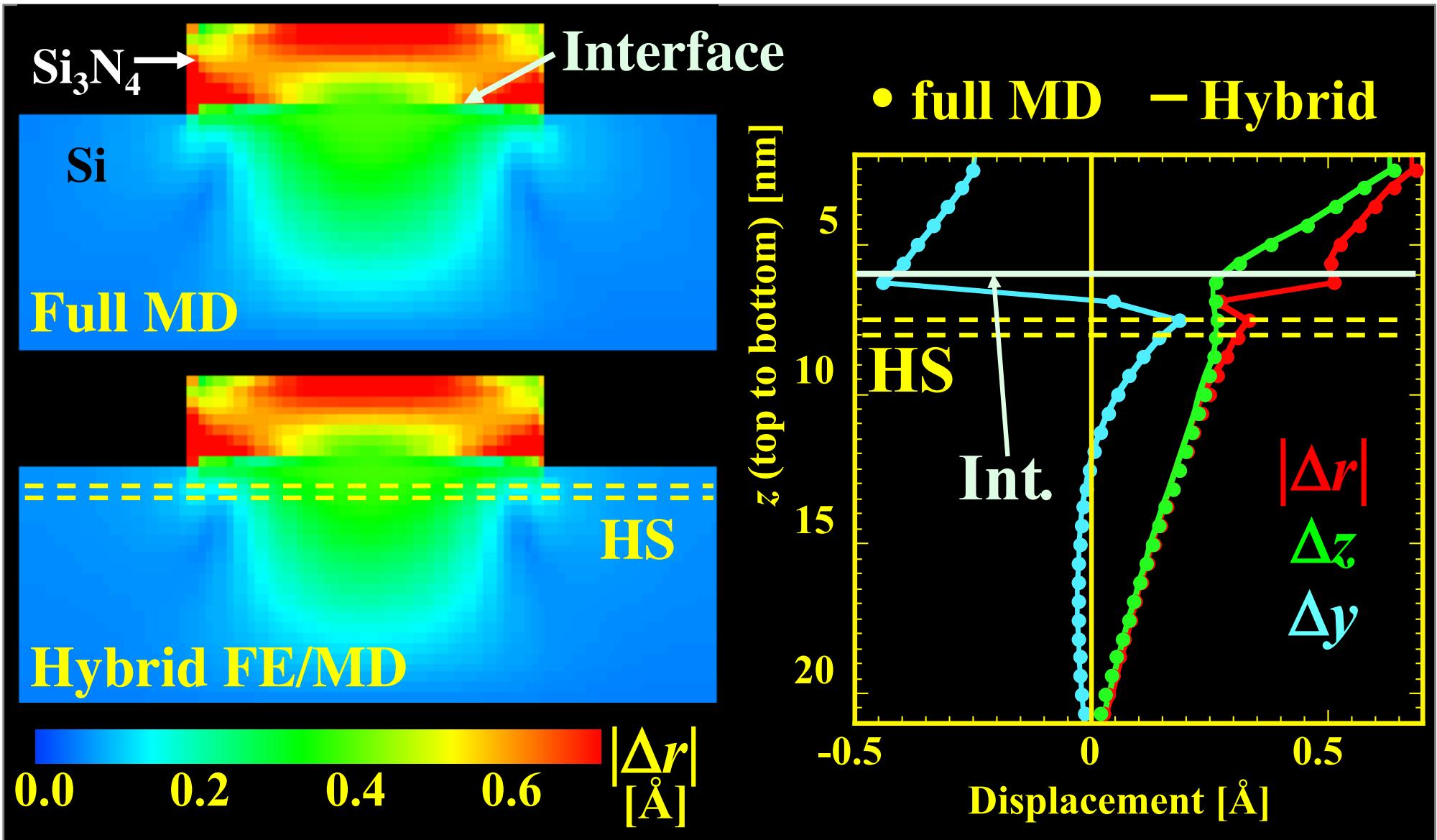
# Hybrid FE/MD Algorithm

- FE nodes & MD atoms coincide in the handshake region
- Additive hybridization

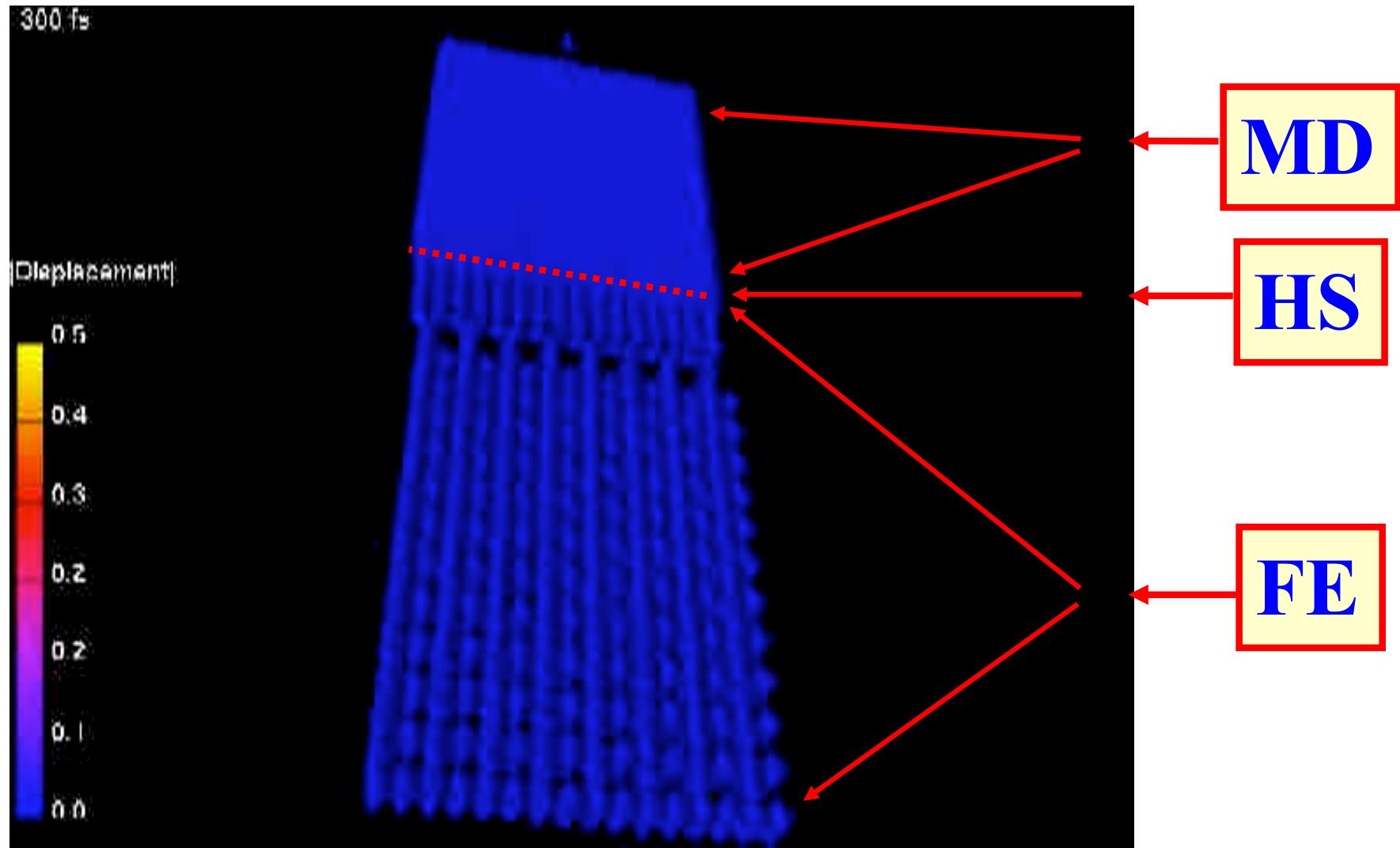


# Si(111)/Si<sub>3</sub>N<sub>4</sub>(0001) Nanopixel

## Displacement from equilibrium positions



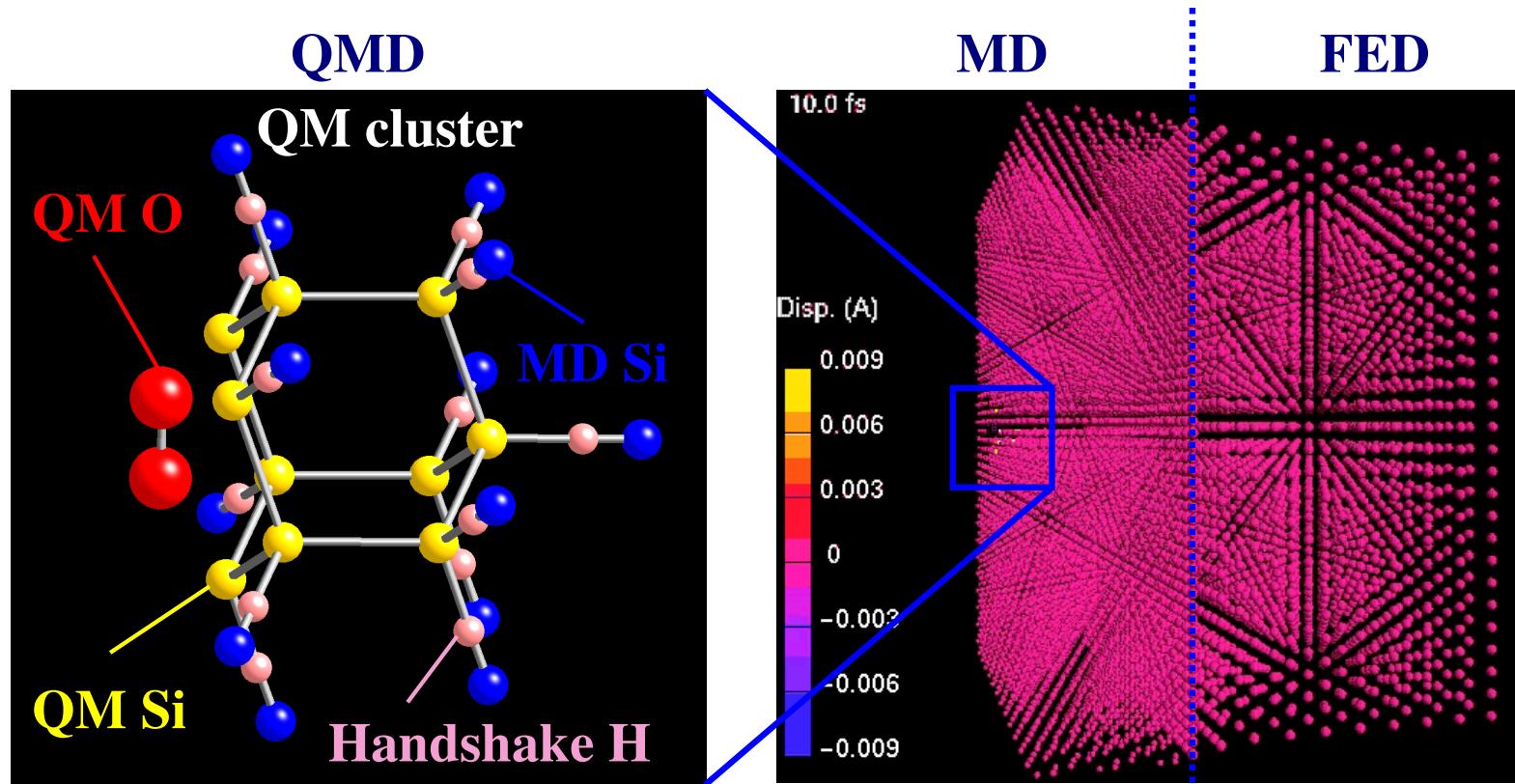
# Dynamics Test & Demonstration: Projectile Impact on Silicon



Waves propagate seamlessly into the FE region

# Application of Multiscale Simulations

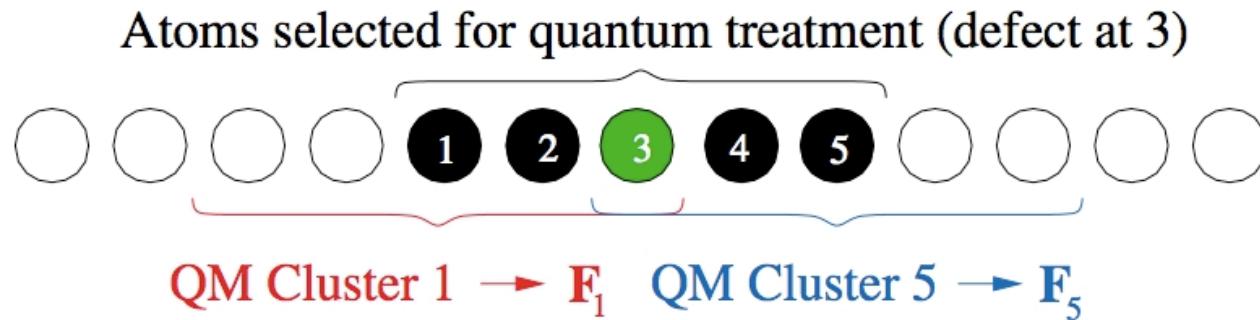
## Oxidation dynamics on Si surface



**QMD/MD/FED:**  
Quantum molecular dynamics/molecular dynamics/finite-element dynamics

# “Learning on the Fly” MD/QM

- Use parameterized interatomic potential, with parameters varying atom-by-atom
- Runtime refit of the parameters in chemically reactive regions by performing small quantum-mechanical calculations



G. Csanyi *et al.*, *Phys. Rev. Lett.* **93**, 175503 ('04); *Nature* **455**, 1224 ('08)

- Use expressive machine-learning (ML) potential like neural network (NN)<sup>1</sup> or Gaussian approximation potential (GAP)<sup>2</sup>
- Active learning to use uncertain quantification (UQ) of the ML potential to re-train the model only when needed<sup>3,4</sup>

<sup>1</sup> J. Behler & M. Parrinello, *Phys. Rev. Lett.* **98**, 146401 ('07); *IJQC* **115**, 1032 ('15)

<sup>2</sup> A. P. Bartok *et al.*, *Phys. Rev. Lett.* **104**, 136403 ('10)

<sup>3</sup> L. Zhang *et al.*, *Phys. Rev. Mater.* **3**, 023804 ('19)

<sup>4</sup> J. Vandermause *et al.*, *arXiv:1904.02042v1a* ('19)

# Coarse Grained Molecular Dynamics

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- Coarse graining:  $\mathbf{u}_j = \sum_{\mu} f_{j\mu} \mathbf{u}_{\mu}, \quad cf. \text{ wavelet smoothing}$
- Reduced (constrained) Hamiltonian → equations-of-motion for  $\mathbf{u}_j$ 's

$$\begin{aligned} E(\mathbf{u}_k, \dot{\mathbf{u}}_k) &= \langle H_{MD} \rangle_{\mathbf{u}_k, \dot{\mathbf{u}}_k} \\ &= \int d\mathbf{x}_{\mu} d\mathbf{p}_{\mu} H_{MD} e^{-\beta H_{MD}} \Delta / Z, \\ \Delta &= \prod_j \delta\left( \mathbf{u}_j - \sum_{\mu} \mathbf{u}_{\mu} f_{j\mu} \right) \delta\left( \dot{\mathbf{u}}_j - \sum_{\mu} \frac{\mathbf{p}_{\mu} f_{j\mu}}{m_{\mu}} \right), \end{aligned}$$

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R. E. Rudd & J. Q. Broughton, *Phys. Rev. B* **58**, R5893 ('98)  
R. Kobayashi et al., *Int'l J. Num. Method Eng.* **83**, 249 ('10)

*cf.* J. Fish *et al.*, *Comput. Methods Appl. Mech. Eng.* **196**, 908 ('07)

# Coarse Graining Using Wavelets

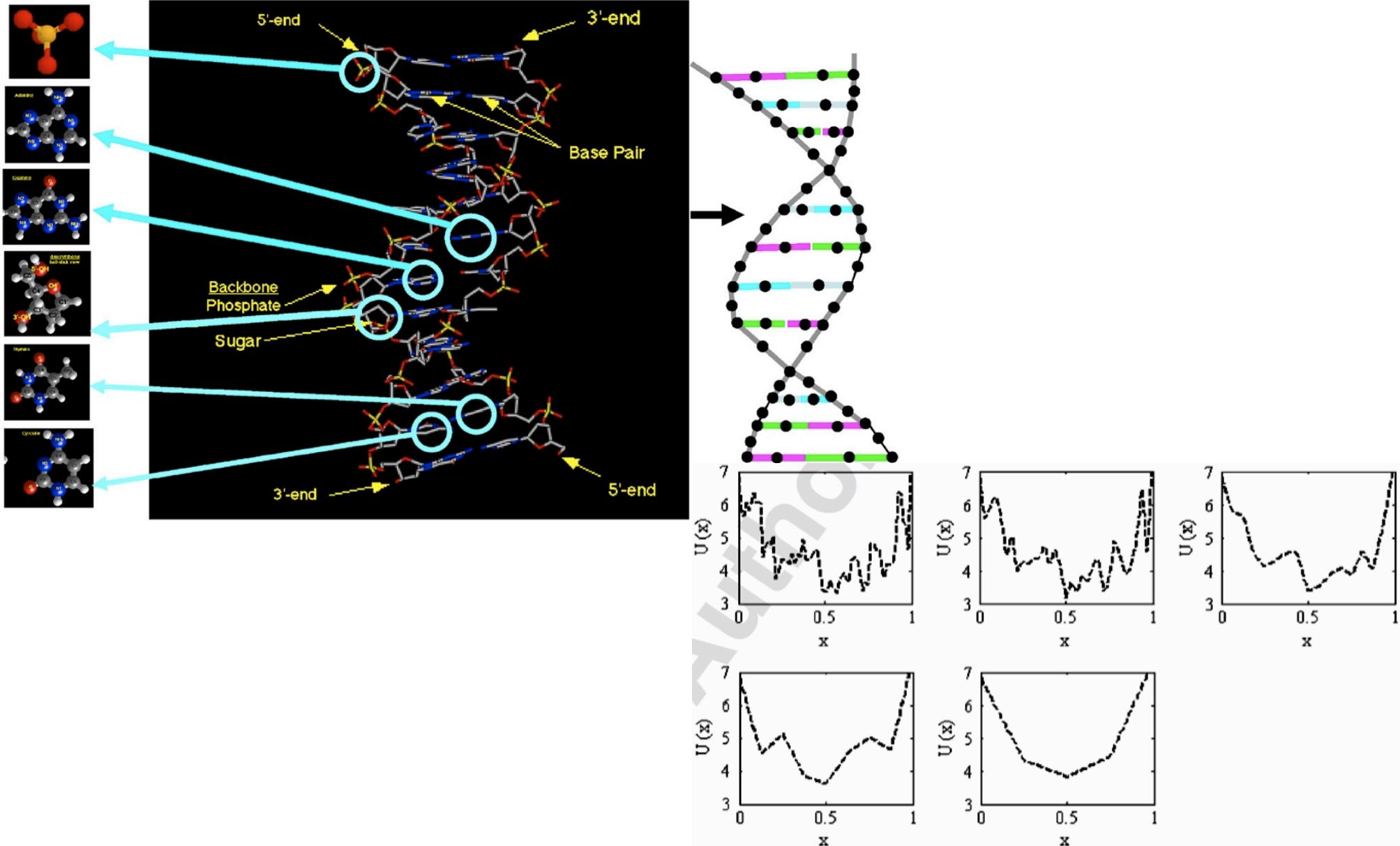


Fig. 11. Effective bond potential based on wavelet multi-scale projection of fine scale bond potential.

J.-S. Chen et al., *Finite Elements in Analysis & Design* 43, 346 ('07)

# Quasicontinuum Method

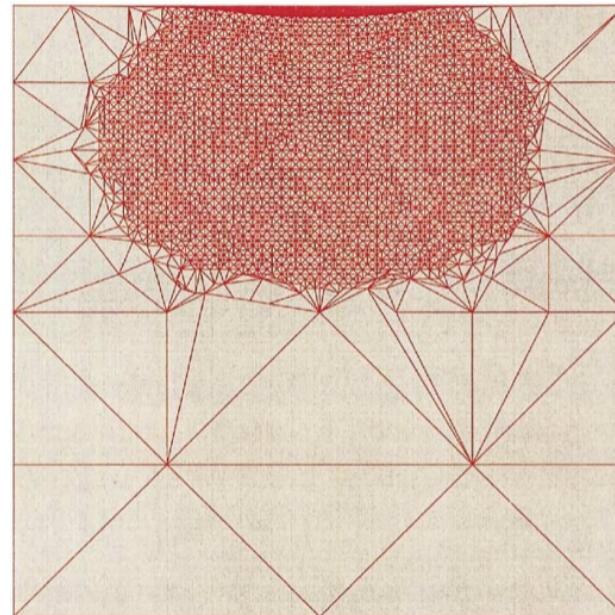
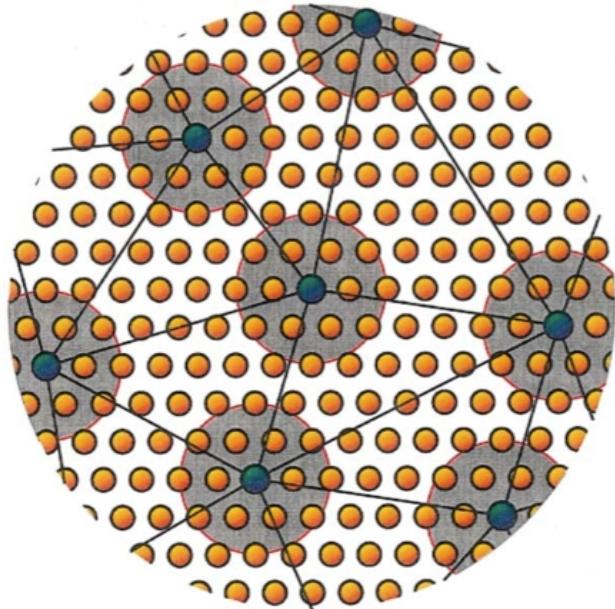
- Piecewise interpolation of the deformation of a selected subset of atoms

$$\mathbf{x}_\mu = \sum_j N_j(\mathbf{x}_\mu) \mathbf{x}_j$$

- Coarse graining as numerical quadrature

$$E_{\text{total}} = \sum_j w_j E_j$$

- Summation weight locally determined by a cluster of atoms centered at the “representative atoms”



V. B. Shenoy *et al.*, *J. Mech. Phys. Solids* **47**, 611 ('99)  
J. Knap & M. Ortiz, *J. Mech. Phys. Solids* **49**, 1899 ('01)

# Linear-Scaling MD/FE Optimization

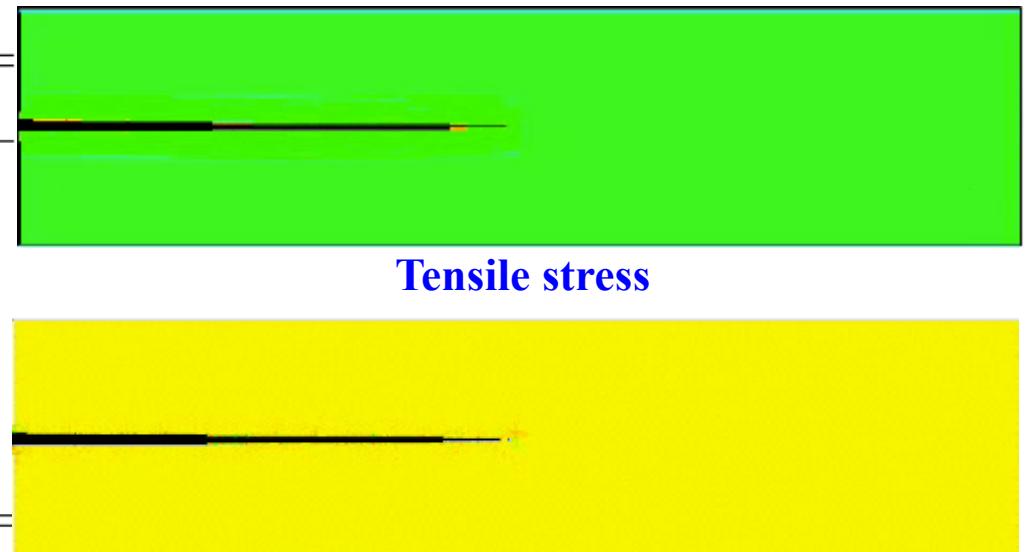
Iterate:

1. Perform a small # of steps of conventional (e.g., CG) energy minimization
2. Perform one step where solid is described by elastic theory
  - a. Calculate the forces acting on the atoms
  - b. Transfer the atomic forces onto a computational grid
  - c. Solve linear elastic eq. with a **multigrid method** to obtain the displacement field
  - d. Get the atomic displacements by interpolating the displacement field
  - e. Move the atoms along the displacement directions

TABLE I. Number of force evaluations  $n_f$  and CPU time  $T$  in seconds for the conjugate gradient (CG) and the linear scaling (SC) method for a divacancy in silicon.

Number of atoms	$n_f$ (CG)	$n_f$ (LS)	$T$ (CG)	$T$ (LS)
510	102	106	0.41	0.50
998	124	106	0.90	0.93
1726	146	109	1.7	1.6
4094	184	115	5.1	4.2
13822	260	115	24.0	14.0
110592	502	115	373.0	135.0
884734	934 	117	5586.0	1147.0

**100 million-atom molecular dynamics simulation  
of a crack tip in GaAs**



S. Goedecker *et al.*,  
*Phys. Rev. B* **64**, 161102(R) ('01)

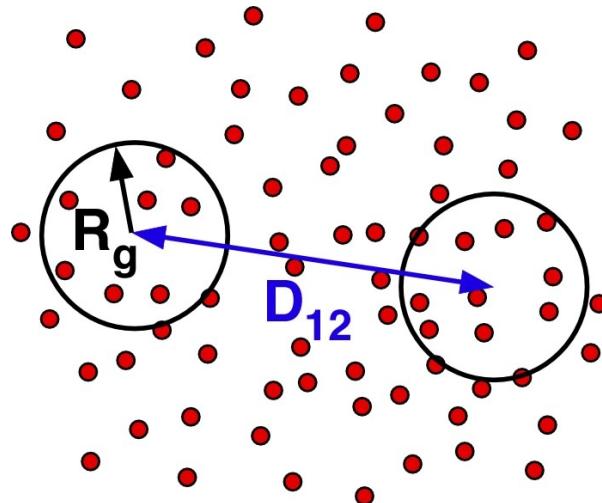
# Dissipative Particle Dynamics

$$\frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{j(\neq i)} \left( \mathbf{f}_{ij}^C + \mathbf{f}_{ij}^D + \mathbf{f}_{ij}^R \right)$$

$$\begin{cases} \mathbf{f}_{ij}^C = a_{ij} (1 - r_{ij}) \hat{\mathbf{r}}_{ij} \Theta(1 - r_{ij}) & \text{coarse interaction} \\ \mathbf{f}_{ij}^D = -g(1 - r_{ij})^2 \Theta(1 - r_{ij}) (\mathbf{v}_{ij} \bullet \hat{\mathbf{r}}_{ij}) \hat{\mathbf{r}}_{ij} & \text{friction} \\ \mathbf{f}_{ij}^R = \sqrt{2gk_B T} (1 - r_{ij}) \Theta(1 - r_{ij}) \text{rnd}_{ij} \hat{\mathbf{r}}_{ij} & \text{random force} \end{cases}$$

- Generalized Langevin equation (Liouville equation & Mori-Zwanzig projection operator) for first-principles derivation of coarse forces

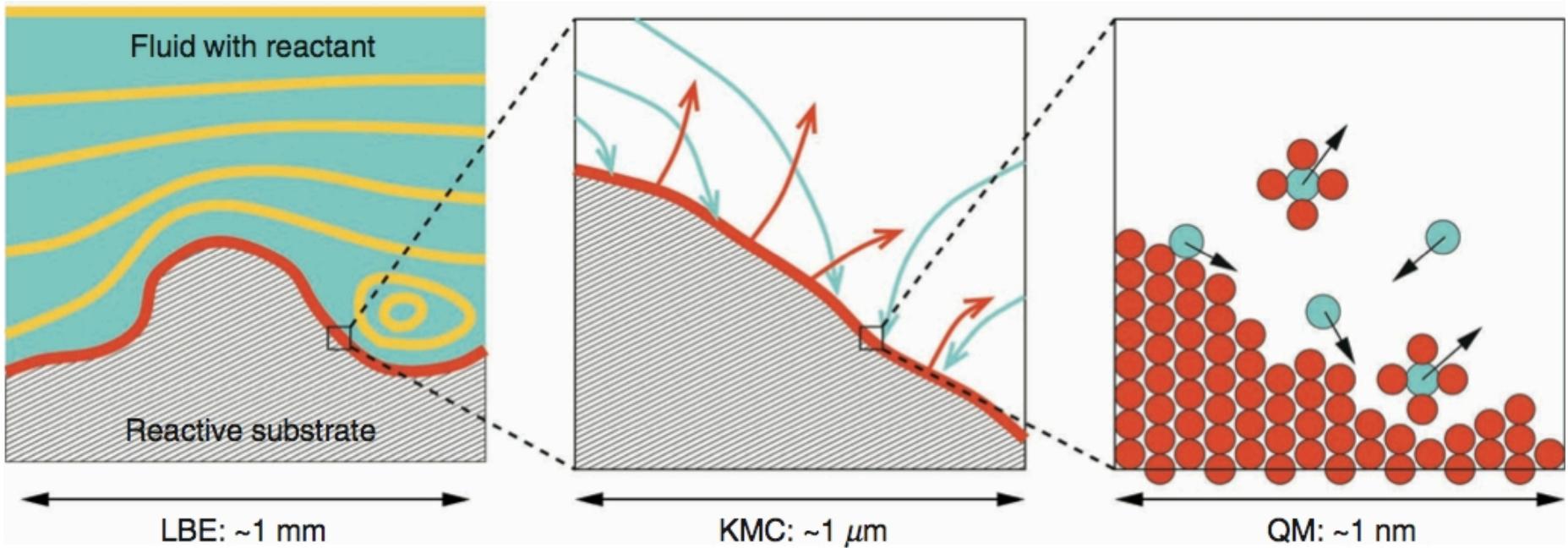
[T. Kinjo & S. Hyodo, *Phys. Rev. E* **75**, 051109 ('07)]



R. D. Groot & P. B. Warren, *J. Chem. Phys.* **107**, 4423 ('97)

# Lattice Boltzmann + Atomistic

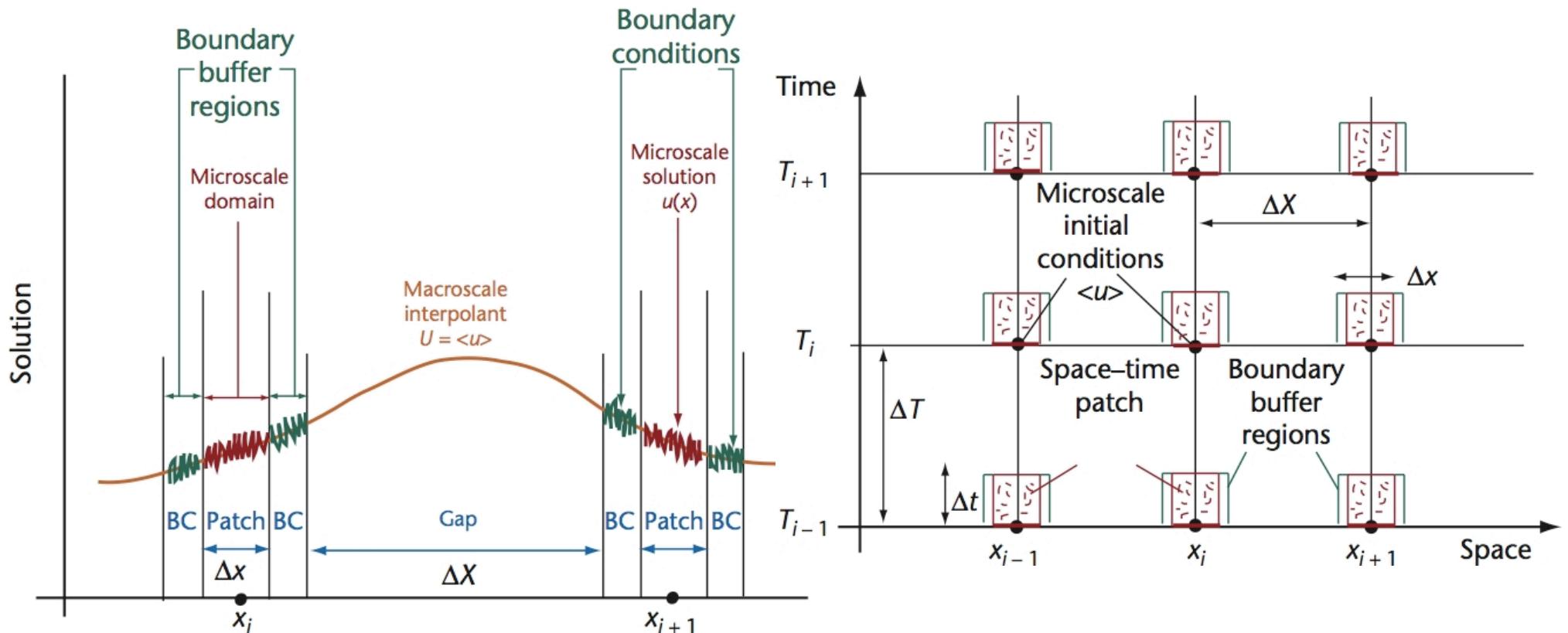
- Coupling fluid dynamics + atomistics/chemical reactions
- Possible breakdown of hydrodynamics at small length scales:  
Boltzmann equation for  $f(x, v, t)$



S. Succi, O. Filippova, G. Smith & E. Kaxiras, *Comp. Sci. Eng.* **3**(6), 26 ('01)  
Y. Kwak et al., *Int'l J. Comput. Sci.* **3**, 579 ('09)

# Spatio-Temporal Interpolation

- Interpolation in both space & time (coarse model can be “equation free”)
- Fine simulations only in small space-time patches



I. G. Kevrekidis, C. W. Gear & G. Hummer, *AIChE. J.* **50**, 1346 ('04)  
J. M. Hyman, *Comp. Sci. Eng.* **7**(3), 47 ('05)