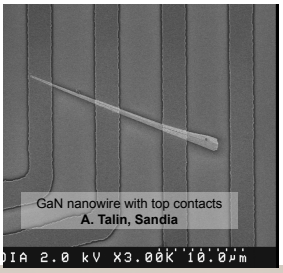
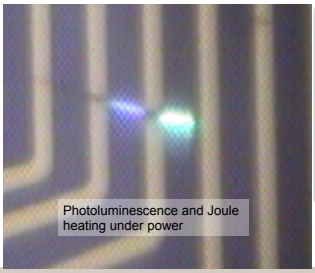
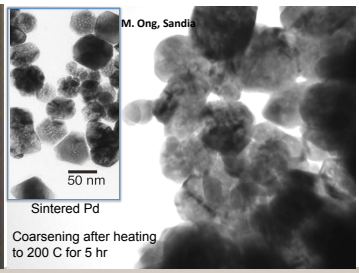
Exceptional service in the national interest

Sandia National Laboratories







We are interested in predicting the outcomes of long time-scale thermal & diffusion processes with atomic detail, e.g.
- [Wagner et al, CMAME,2008]
- [Templeton et al,MSMSE,2010]

We have developed methods for time integration:
- fractional-step integration
- multiple time-scale integration
- projective integration

as well as parallel implementations of parallel replica dynamics, temperature accelerated dynamics, etc.

Time-scale issues in molecular dynamics-finite element coupling applications

R. Jones, J. Templeton, G. Wagner

Fractional Step Integration

MD/FE thermal coupling requires a stable interleaving of integrators for the molecular and coarse scale dynamics

[J. Templeton et al, in preparation]

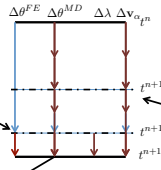
Atoms contribute to nodal heat equation

$$\sum_J \frac{\partial}{\partial t}(M_{IJ}\theta_J) = \sum_J K_{IJ}\theta_J + 2\sum_\alpha N_{I\alpha}\mathbf{v}_\alpha \cdot \left(\mathbf{f}_\alpha^{MD} + \frac{1}{2}\mathbf{f}_\alpha^{\lambda}\right)$$

Heat at nodes affects MD energy through a spatial thermostat

Gear update for FE dynamics, predictor/corrector requires:

$$\dot{\theta}^{FE} = M_{IJ}^{-1}K_{IK}\theta_K$$



Velocity-Verlet update for MD, two-step update requires:

$$\dot{\mathbf{v}}_\alpha = m_\alpha^{-1}\mathbf{f}_\alpha^{MD}$$

$$\Delta t\lambda < 1$$

Update Lagrange multipliers after the prediction phase by solving the non-linear equation:

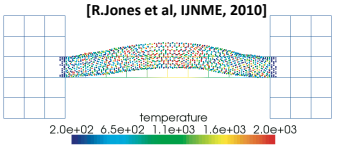
$$\Delta t \sum_\alpha N_I^\alpha K_\alpha \sum_J N_J^\alpha \lambda_J - \frac{\Delta t^2}{4}\sum_\alpha N_I^\alpha K_\alpha \left(\sum_J N_J^\alpha \lambda_J\right)\left(\sum_K N_K^\alpha \lambda_K\right) = R_I^\alpha$$

Apply resulting force at three time increments: t^n, $t^{n+1/2}$, and $t^{n+1,*}$

Multiple Time-scale Integration

Given the relative thermal properties of electrons and phonons, an efficient coupling scheme needs to operate on two disparate timescales

[R.Jones et al, IJNME, 2010]



Two temperature model:

$$\frac{d}{dt}\theta_e = -(\theta_e - \theta_p)$$

Assume short & long timescales:

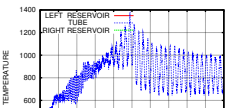
$$\frac{d}{dt} \rightarrow \frac{\partial}{\partial t} + \epsilon\frac{\partial}{\partial t_2}$$

Expand and substitute:

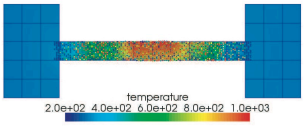
$$\frac{\partial}{\partial t_2}\theta_{e,1} = -\theta_{e,0} - \frac{\partial}{\partial t}\theta_{e,0} + \theta_p$$

Result : electrons interact with filtered/long time-scale phonon evolution

$$\frac{\partial}{\partial t}\theta_{e,0} = -(\theta_{e,0} - \langle\theta_p\rangle)$$



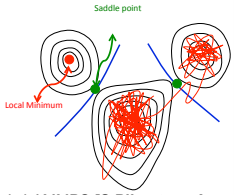
Laser heating of a CNT connect to thermal reservoirs



Accelerated MD Methods

Accelerated MD methods focus on infrequent events that drive dynamics (e.g. atom-hopping)

- Ignore long periods of thermal vibration within energy basins



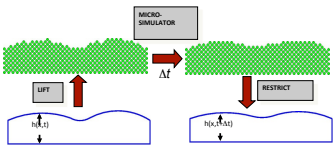
Methods have been implemented in Sandia's LAMMPS **[S.Plimpton,, A. Thompson, P. Crozier]** code:

- Nudged Elastic Band (NEB), Parallel Replica Dynamics (PRD), Temperature Accelerated Dynamics (TAD)
- Innovations in parallelization of methods
- New features can be used with any LAMMPS interatomic potential
- Open source release to broad research community

See http:/lammps.sandia.gov
(and http://www.sandia.gov/~sjplimp/spparks.html)

Projective Integration

To model surface diffusion with the Equation-Free Method [I. Kevrekidis et al, 2003], fine/coarse scale descriptions are used to extend to longer timescales



Approximate: $\frac{\partial h}{\partial t} \approx \frac{1}{\Delta t}\left(h(t+\Delta t) - h(t)\right)$

Project: $h(t+\Delta T) = h(t) + \Delta T\frac{\partial h}{\partial t}$

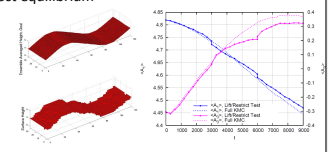
(1) Use fine-scale simulations as "computational experiments" to get approximate course-scale time derivatives
(2) Project coarse scales in time over longer timestep, and reinitialize fine scales

An Improved Lift Operator: The Maximum Entropy Method

[G. Wagner et al, *Int. J. Multiscale Comp. Eng.*, 2010]
[J. Deng et al, in preparation]

The lift operator must preserve higher-order system statistics (like spatial correlations) to replicate dynamics but this is problem specific & difficult in higher dimensions

The goal is to constrain only the coarse scale values of interest, but allow other variables to come into correct equilibrium



Given "goal" average profile shape (top), generate many individual realizations (bottom) that, when ensemble averaged, reproduce the goal profile while also preserving the correct dynamics (right).

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
SAND No. 2011-XXXXP