UNIVERSITÄT SIEGEN

PD Dr.-Ing. habil. B. Eidel
Heisenberg-Fellow (DFG)
Chair of Computational Mechanics
Department of Mechanical Engineering

Heisenberg-Programm
Deutsche Forschungsgemeinschaft

FIRE: Accelerated Energy-Minimization in Atomistic FEM based on Acceleration, Inertia and Numerical Quenching

• Motivation and Goal

Energy minimization in atomic simulations at zero temperature is used to find the (inherent) equilibrium structure of a solid without the "noise" of thermal vibrations.

The goal is to reformulate an algorithm with superior convergence for flat energy landscapes and instability problems for the Cluster-Based QC Method as an examplary atomistic finite element method.

In [4] a simple MD scheme for structural relaxation was proposed. The algorithm dubbed FIRE for *Fast Inertial Relaxation Engine* (FIRE) relies on inertia. The strategy is to descent to an energy-minimum following an equation of motion by

$$\dot{\boldsymbol{v}}(t) = 1/m\, \boldsymbol{F}(t) - \gamma(t)|\boldsymbol{v}(t)| \left[\hat{\boldsymbol{v}}(t) - \hat{\boldsymbol{F}}(t)\right], \qquad (1)$$

with mass m, velocity $\boldsymbol{v} = \dot{\boldsymbol{x}}$, force $\boldsymbol{F} = -\nabla E^{\mathrm{QC}}(\boldsymbol{x})$, and where the hat denotes a unit vector.

• Strategy

– Accelerate in a direction that is "steeper" than the current direction of motion via the function $\gamma(t)$.

– Avoid uphill motion the algorithm stops as soon as the power $P(t) = \boldsymbol{F}(t) \cdot \boldsymbol{v}(t)$ becomes negative.

– Choose parameter $\gamma(t)$ appropriately; not too large, because the current velocities carry information about the reasonable 'average' descent direction and energy scale, [4].

– The numerical treatment: Use an MD integrator providing the propagation of the trajectories due to conservative forces. Readjust continuously the MD trajectories by a mixing rule of the velocities according to

$$\boldsymbol{v} \to (1-\alpha)\boldsymbol{v} + \alpha\hat{\boldsymbol{F}}|\boldsymbol{v}|\,, \qquad \alpha = \gamma\Delta t \qquad (2)$$

following from an Euler-step in eq. (1) with time step size Δt.

• Propagation rules for the FIRE algorithm

initialization: set Δt, $\alpha = \alpha_{\mathrm{start}}$, the vectors $\boldsymbol{x}$ and $\boldsymbol{v} = \boldsymbol{0}$.

1. MD integrator: calculate $\boldsymbol{x}$, $\boldsymbol{F} = -\nabla E^{\mathrm{QC}}(\boldsymbol{x})$ and $\boldsymbol{v}$ using any common MD integrator (here: Velocity Verlet); check for convergence.
2. calculate force power $P = \boldsymbol{F} \cdot \boldsymbol{v}$.
3. set $\boldsymbol{v} \to (1-\alpha)\boldsymbol{v} + \alpha|\boldsymbol{v}|\hat{\boldsymbol{F}}$.
4. if $P > 0$ and the number of steps since P was negative is larger than $N_{\min}$, increase the time step $\Delta t \to \min(\Delta t f_{\mathrm{inc}}, \Delta t_{\max})$ and decrease $\alpha \to \alpha f_\alpha$.
5. if $P \leq 0$, decrease time step $\Delta t \to \Delta t f_{\mathrm{dec}}$, freeze the system $\boldsymbol{v} \to \boldsymbol{0}$, and set α back to α_{start}.
6. Return to MD integrator.

Here: $N_{\min} = 5$, $\alpha_{\mathrm{start}} = 0.1$, $f_{\mathrm{inc}} = 1.1$, $f_{\mathrm{dec}} = 0.5$, $f_\alpha = 0.99$.

• Compression of a Micro-Pillar

An fcc single-crystalline pillar subject to axial compression exhibits plastic deformation localizing in a shear band.

The novel FIRE minimizer is tested against the Steepest Descent (SD) method, a nonlinear version of the Conjugate Gradient (CG) method and the Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm. The total deformation range can be decomposed into three parts, I-III:

I. Surface relaxation. The energy landscape is 'flat'. FIRE by virtue of inertia passes local minima towards the global minimum much faster than other algorithms.

II. Elastic compression up to 7%. FIRE is much faster than L-BFGS. CG and SD are not competitive.

III. Material instability: bifurcation into deformation localization (shear-banding). CG and SD do not converge. FIRE is faster than L-BFGS.

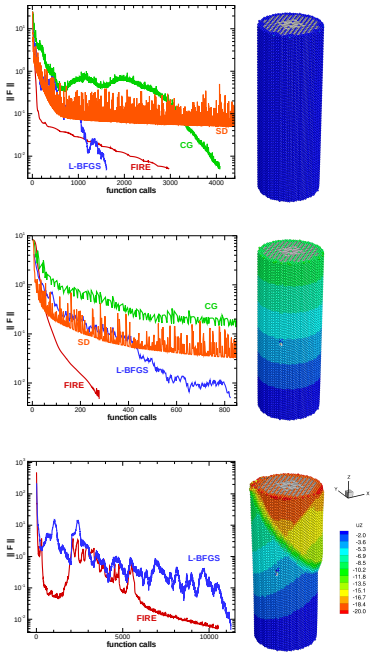

Fig. 1. Convergence diagrams for different optimizers at characteristic deformation stages of the nanopillar (left), contour plots for axial displacement component u_z [Å] (right).

Conclusion

The novel optimizer based on acceleration and inertia shows in its adaption to a variationally consistent, fullynonlocal QC method a competitive and partially superior behavior compared with state-of-the-art optimizers like L-BFGS. These promising results suggest further investigations and the use of the algorithm for various other models and applications.

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B. Eidel
University of Siegen, Chair of Computational Mechanics
University of Duisburg-Essen, Institute of Mechanics

A. Stukowski
Materials Modeling
TU Darmstadt