Inter-scale Model Discrepancy

A typical Bayesian approach to reduce model discrepancy seeks to minimize bias and maximize identifiability of calibration parameters (Ling et al., J. Comput. Phys. 276, 2014) via introduction of explicit additive terms to adjust model response or parameters.

Alternative approach: introduce an inter-scale discrepancy formulation that involves the BU and/or TD mappings, having a physical basis.

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Recent work led by Aaron Tallman

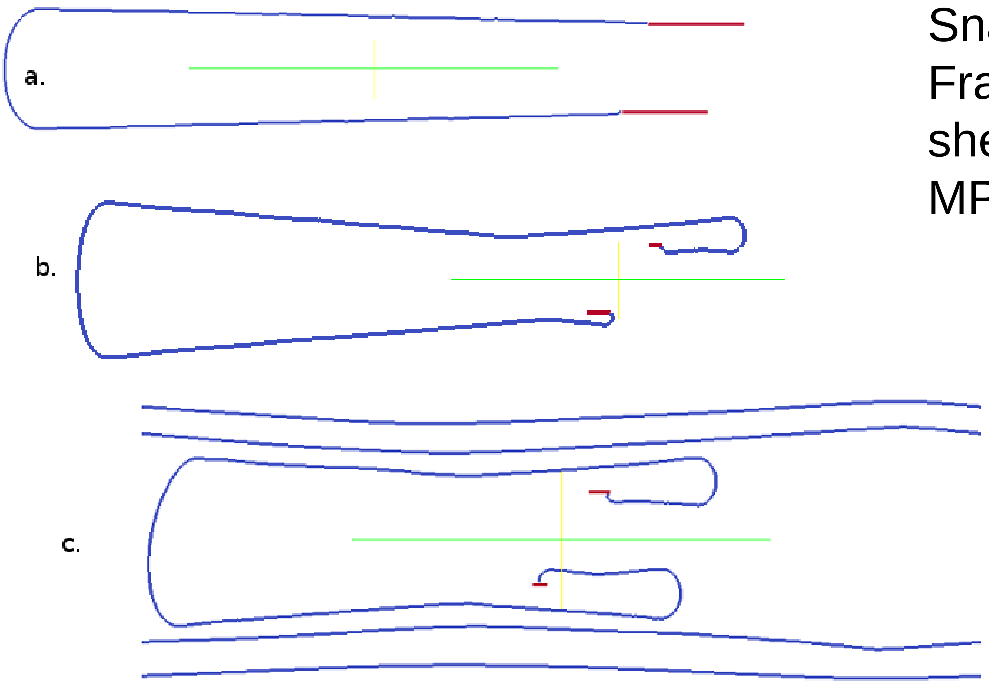
Model Discrepancy Layer

- The previously used top-down (TD) and bottom-up (BU) likelihood functions are augmented with an inter-scale discrepancy layer.
- The model discrepancy layer involves a single parameter: the thermal slip resistance, s_t

$$s_{t,BU} = C_p \, s_{t,TD} \quad , \quad C_p \approx 2$$

Motivated by reduced stress necessary to activation Frank-Read sources in dislocation networks, after Gröger and Vitek, Phil Mag Lett 87, 2007.

DDD Simulations of a Frank-Read Source



Snapshots of DDD simulations of Frank-Read sources under applied shear stress of 500 MPa (a.), 750 MPa (b.), and 1000 MPa (c.).

Initial dislocation density ~ 3x10^{10} /m^2
Lower than 10^{12} /m^2 value considered by Vitek.
At higher dislocation densities, attraction of dislocation dipoles would further reduce stress necessary for F-R source operation

The DDD simulations of a Frank-Read source are carried out using a prismatic dislocation loop. The glissile portions of the loop are initially pure edge dislocation segments on $\frac{1}{2}\langle 111\rangle\{110\}$ slip systems.

The simulations are carried out to examine whether or not the screw segments that form as the dislocation bows out will inhibit the formation of glide loops. This step is identified as critical to the feasibility of the explanation provided by Gröger and Vitek (2007).

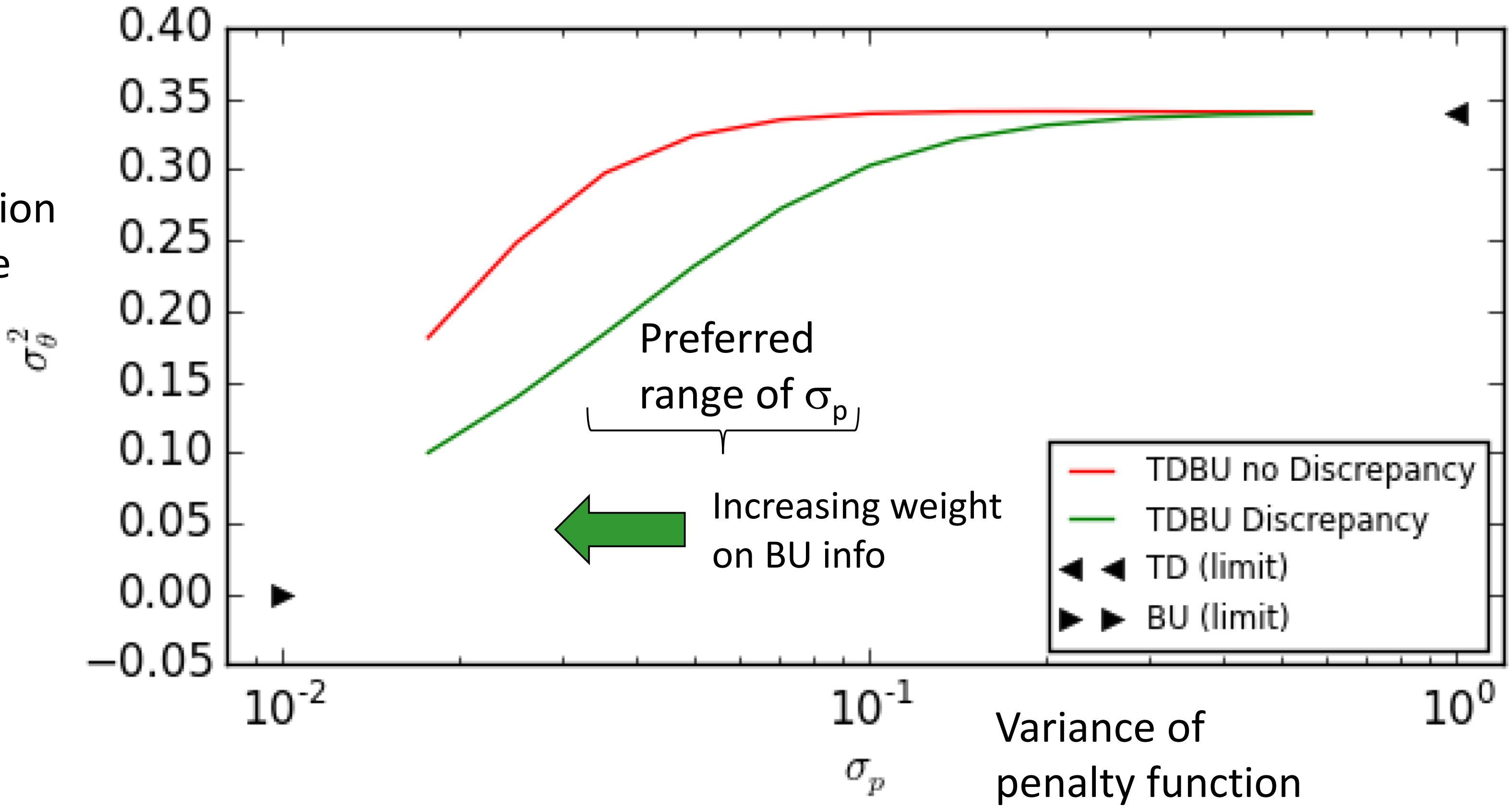
As a result…

The original and discrepancy adjusted reference estimates used in the BU penalization.

$\hat{\boldsymbol{\theta}}_{\mathrm{BU}}^{ref}$	$\dot{\gamma}_0$	ΔF_g	p	q	s_t
Original	$3.19\times10^7 s^{-1}$	0.57 eV	0.67	1.18	1040 MPa
Discrepancy Adjusted	$3.19\times10^7 s^{-1}$	0.57 eV	0.67	1.18	520 MPa

Calibration Variance as a Function of the Penalty Parameter

Normalized calibration variance decreases significantly with inter-scale discrepancy layer



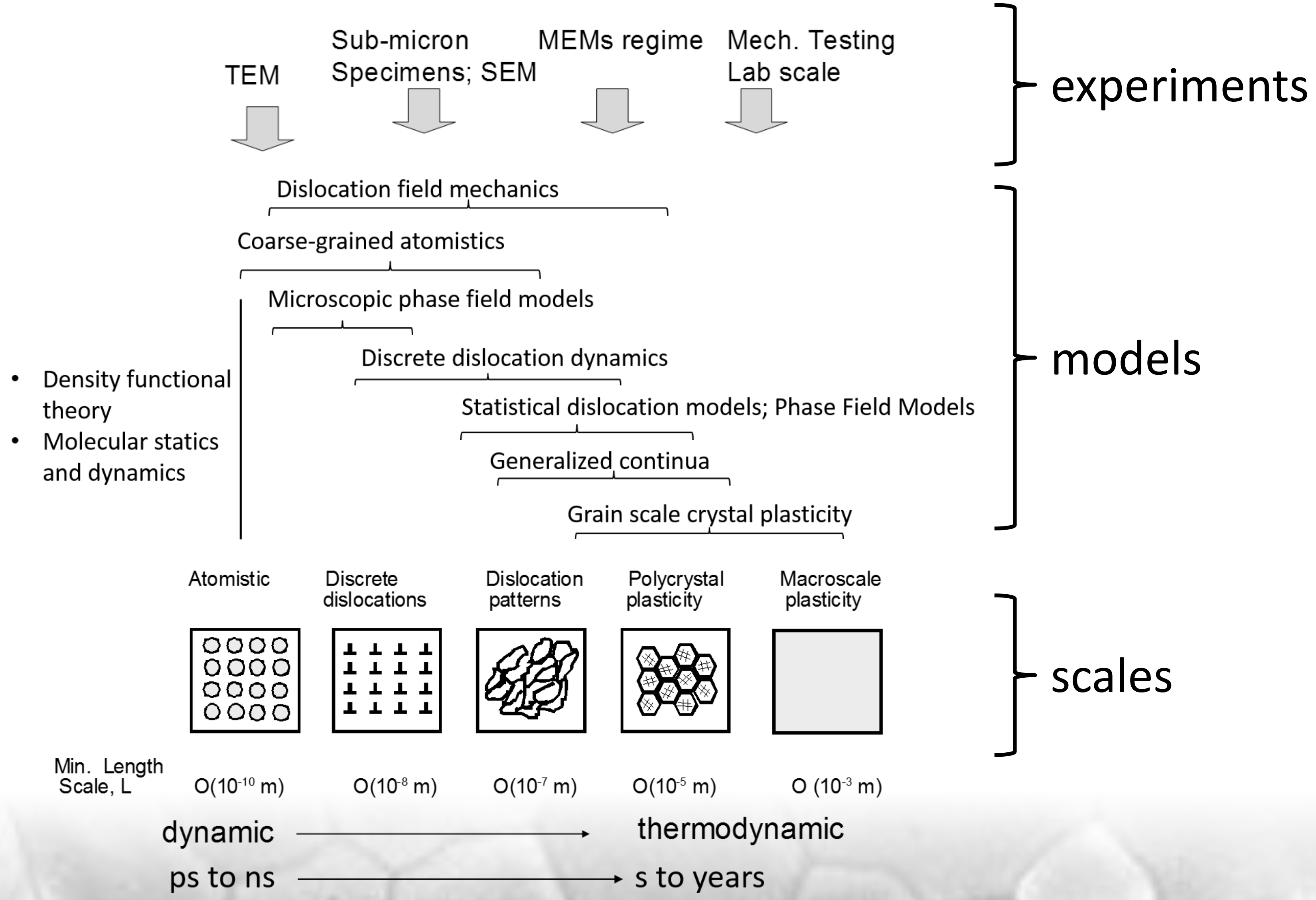
Calibration variance

Preferred range of σ_p

Increasing weight on BU info

Variance of penalty function

The Challenge of HMMs



TEM

Sub-micron Specimens; SEM

MEMs regime

Mech. Testing Lab scale

experiments

Dislocation field mechanics

Coarse-grained atomistics

Microscopic phase field models

Discrete dislocation dynamics

Statistical dislocation models; Phase Field Models

Generalized continua

Grain scale crystal plasticity

- Density functional theory
- Molecular statics and dynamics

models

Min. Length Scale, L	Atomistic	Discrete dislocations	Dislocation patterns	Polycrystal plasticity	Macroscale plasticity
	O(10^{-10} m)	O(10^{-8} m)	O(10^{-7} m)	O(10^{-5} m)	O (10^{-3} m)

scales

dynamic → thermodynamic

ps to ns → s to years

Scale Bridging Methods – HMMs

Panchal, Kalidindi, McDowell, Computer-Aided Design, 2013

Length Scale	Time Scale	Models	Examples of Scale Bridging Approaches	Primary Sources of Uncertainty
2 nm	NA/ ground state	First principles, e.g., Density Functional Theory (DFT)		Assumptions in DFT method, placement of atoms
			Quantum MD	
200 nm	10 ns	Molecular dynamics (MD)		Interatomic potential, cutoff, thermostat and ensemble
			Domain decomposition, coupled atomistics discrete dislocation (CADD), coarse grained MD, kinetic Monte Carlo	Attenuation due to abrupt interfaces of models, passing defects, coarse graining defects
2 μm	s	Discrete dislocation dynamics		Discretization of dislocation lines, cores, reactions and junctions, grain boundaries
			Multiscale crystal plasticity	Averaging methods for defect kinetics and lattice rotation
20 μm	1000 s	Crystal plasticity, including generalized continuum models (gradient, micropolar, micromorphic)		Kinetics, slip system hardening (self and latent) relations, cross slip, obstacle interactions, increasing # adjustable parameters
			RVE simulations, polycrystal/composite homogenization	RVE size, initial and boundary conditions, eigenstrain fields, self-consistency
200 μm	Days	Heterogeneous FE with simplified constitutive relations		Mesh refinement, convergence, model reduction
			Substructuring, variable fidelity, adaptive	Loss of information, remeshing error,

Opportunities and Challenges

Concurrent Multiscale Modeling

- Address model form uncertainty to facilitate concurrency
- Address complex, configuration/environment dependent phenomena
- Intrusive/embedded methods in HPC

Hierarchical Multiscale Modeling

- Emphasis to date: parameter uncertainty, variance of QoIs. Should shift more attention to:
    - Identification of number of models/scales
    - Uncertainty of linking algorithms and model calibration
    - Linking strategies considered as a part of model form, i.e., uncertainty of the configuration of the system and information flow
- Utility of bottom-up vs top down information

Thanks!