"From defects to cracks: Optimal scaling laws in ductile fracture"

Michael Ortiz
Frank and Ora-Lee Marble Professor
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We perform an optimal-scaling analysis of ductile fracture in metals. We specifically consider the deformation up to failure of a slab of finite thickness subject to monotonically-increasing normal opening displacements on its surfaces. We show that ductile fracture in metals can be understood as the net outcome of two competing effects: the sublinear growth characteristic of the hardening of metals and strain-gradient plasticity. We also put forth physical arguments that identify the intrinsic length of strain-gradient plasticity and the critical opening displacement for fracture. We show that, when fracture properties are renormalized in a manner suggested by the optimal scaling laws, the experimental data tends to cluster---with generous allowances made for experimental scatter---within bounds dependent on the hardening exponent but otherwise material independent. Buoyed by this success, we attempt to apply the same theory to the ductile fracture of polymers. Surprisingly, we find that strain-gradient elasticity is too rigid and does not allow for the commonly observed crazing mechanism of ductile fracture in polymers. We show that, a generalization based on fractional strain-gradient elasticity relaxes the theory sufficiently to allow for crazing. We again derive optimal scaling laws that supply a link between macroscopic and micromechanical properties. Finally, we demonstrate the scope and fidelity of the model by means of an examples of application, including simulations of hypervelocity impact of metallic plates and Taylor-impact experiments of polyurea~1000 rods.

Ideal Strength, Elastic Anisotropy and Dislocation Plasticity: the Curious Case of Gum Metal

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Abstract

In 2003, researchers at Toyota introduced a TiNb based alloy that they named Gum Metal. The alloy displays super strength, super elasticity and considerable ductility. In fact the alloy's observed strength approaches the its ideal strength. These properties fully emerge only after extensive cold swaging. However, post-deformation microstructures reveal few (if any) dislocations. These observations (amongst others) led Toyota researchers to claim that Gum Metal is the first bulk engineering alloy to deform at ideal strength. The interesting properties of Gum Metal beg the question: Where are the dislocations? In this talk, I will present our studies of dislocations within Gum Metal, and discuss how the elastic anisotropy that emerges near a concentration driven phase transformation results in easy pinning and extreme spreading of the dislocation cores, ultimately leading to the impressive mechanical properties of Gum Metal.

Large-scale electronic structure calculations and studies on defects

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Defects play a crucial role in influencing the macroscopic properties of solids—examples include the role of dislocations in plastic deformation, dopants in semiconductor properties, and domain walls in ferroelectric properties. These defects are present in very small concentrations (few parts per million), yet, produce a significant macroscopic effect on the materials behavior through the long-ranged elastic and electrostatic fields they generate. The strength and nature of these fields, as well as other critical aspects of the defect-core are all determined by the electronic structure of the material at the quantum-mechanical length-scale. Hence, there is a wide range of *interacting* length-scales, from *electronic structure to continuum*, that need to be resolved to accurately describe defects in materials and their influence on the macroscopic properties of materials. This has remained a significant challenge in multi-scale modeling, and a solution to this problem holds the key for *predictive* modeling of complex materials systems.

In an attempt to address the aforementioned challenge, this talk presents the development of a *seamless* multi-scale scheme to perform electronic structure calculations at macroscopic scales. The key ideas involved in its development are (i) a real-space variational formulation of electronic structure theories, (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure. This multi-scale scheme has enabled, for the first time, calculations of the electronic structure of multi-million atom systems using orbital-free density-functional theory, thus, paving the way for an accurate electronic structure study of defects in materials. The accuracy of the method and the physical insights it offers into the behavior of defects in materials is highlighted through studies on vacancies and dislocations. Current efforts towards extending this multi-scale method to Kohn-Sham density functional theory will also be presented, which include: (i) the development of higher-order adaptive finite-element formulation for efficient real-space Kohn-Sham DFT calculations; (ii) the development of a linear-scaling approach that is applicable to both insulating and metallic systems.

Electronic and plasmonic phenomena at graphene grain boundaries

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Line defects that are omnipresent in graphene films fabricated with chemical vapor deposition method (CVD) were studied with scattering-type scanning near-field microscope (sSNOM) –a unique technique allowing efficient excitation and high-resolution imaging of graphene plasmons [1,2]. The characteristic sSNOM features of line defects are plasmonic twin fringes, which are generated due to interference between surface plasmons of graphene launched by a scanning probe and reflected by the line defects. The twin fringes allow us to visualize and distinguish various types of line defects including cracks, wrinkles, and most interestingly grain boundaries. Unlike other line defects, grain boundaries are in the atomic length scale. Therefore it remains challenging to characterize their physical properties with traditional methods. I will show that our technique together with modeling and analysis provide a convenient way to uncover the electronic and plasmonic properties associated with grain boundaries in graphene [3].

[1] Z. Fei et al. Nano Lett. 11(11), 4701-4705 (2011).

[2] Z. Fei et al. Nature 487, 82–85 (2012).

[3] Z. Fei et al. Nature Nanotech. 8, 821–825 (2013).

Towards the ab-initio study of defects: Coarse-graining Density Functional Theory

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Crystal defects, though present in relatively minute concentrations, play a significant role in determining macroscopic properties. The accurate characterization of defects represents a unique challenge since both the electronic structure of the defect core as well as the long range elastic field need to be resolved simultaneously. Unfortunately, accurate ab-initio electronic structure calculations are limited to a few hundred atoms, which is orders of magnitude smaller than that necessary for a complete description at physically relevant concentrations.

We present a real-space formulation for coarse-graining Density Functional Theory [1] that significantly speeds up the analysis of crystal defects without appreciable loss of accuracy. The proposed technique consists of two steps. First, we develop a linear-scaling method [1, 2] in terms of quantities amenable to coarse-graining. Next, we introduce a spatial approximation scheme which is adapted so as to furnish fine resolution where necessary and to coarsen elsewhere. We validate the formulation through selected examples.

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Symposium on New Developments in Defects Mechanics

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Dislocation emission at grain boundaries studied by nonlinear field projection

KYUNG-SUK KIM

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Abstracts

The intrinsic strength of a grain boundary at the nanometer scale has been traditionally considered to be governed by the strength of a dislocation emission at a stress concentration point, or of grain boundary cleavage separation. However, on the contrary, our recent extensive MD simulations reveal that the strength is primarily governed by mechanisms of cooperative dislocation emission. In this study, we found an interesting symmetry-breaking bifurcation mechanism of simultaneous multiple dislocation emission, which governs the ductility as well as the strength of the grain boundary. This cooperative mechanism explains why local-strengthening segregates such as bismuth or lead atoms in copper weaken the global strength of the grain boundary. This mechanism is verified by MD simulations for the strength of <110> symmetric tilt angle FCC copper (or nickel) grain boundaries with and without lead doping for the whole range of tilt angles. The simulations show that the lead dopants inhibit the anti-symmetric mode of the cooperative dislocation emission, and in turn embrittle the grain boundary. For both computational and experimental studies of the nanometer-scale grain-boundary strengthening mechanism, new algorithms of interior and exterior nonlinear field projections are introduced.

Dynamic Eshelby Micromechanics
(with inertia effects)

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University of California, San Diego

Abstract

"Eshelby micromechanics" can be called the micromechanics based on the two celebrated Eshelby papers: The "force on an elastic singularity", or "Eshelby force" (1951), (associated with Noether's theorem and conserved integrals) and the ellipsoidal inclusion with transformation strain (1957) where the Eshelby tensor allows for the solution of inhomogeneities as well. Both of these Eshelby micromechanics building blocks are extended to dynamics with inertia. It will be presented that for *self-similarly* expanding ellipsoidal inclusions the constant stress Eshelby property in the interior holds, and that the dynamic Eshelby tensor (for self-similar motion) is obtained analytically (which leads to the analytical solutions of dynamically expanding inhomogeneities). The elastodynamic evolution of moving defects (dislocations, expanding inclusion and inhomogeneity boundaries) is governed by the dynamic conservation laws (*J*, *L*, *M* integrals) from Noether's theorem yielding the "kinetic relations" due to inertia. Interaction of defects and macroscopic damage evolution by the conserved integrals in asymptotic homogenization will also be discussed.

References:

X. Markenscoff, Evolution of Growth of interacting near-by micro-Cavitie and macroscopic Damage Amplification, *J. Math. Mech. Sol*,**19**,71-81, 2014.

Annular Inhomogeneities with Eigenstrain and Interphase Modeling.

Xanthippi Markenscoff
UCSD

Two and three-dimensional analytical solutions for an inhomogeneity annulus/ring (of arbitrary thickness) with eigenstrain are presented. The stresses in the core may become tensile (for dilatational eigenstrain in the annulus) depending on the relative shear moduli. For shear eigenstrain, an "interface rotation" and rotation jumps at the interphase also occur, consistent with the Frank-Bilby interface model. A Taylor series expansion for small thickness of the annulus is obtained to the second-order as to model thin interphases, with the limit agreeing with the Gurtin-Murdoch surface membrane, but also accounting for curvature effects.. The Eshelby "driving forces" on a boundary with eigenstrain are calculated, and for small, but finite, interphase thicknesses they account for the interaction of the two interfaces of the layer, and the next order term may induce instabilities, for some bimaterial combinations, if it becomes large enough to render the driving force zero. It is also proven that for 2-D inhomogeneities with eigenstrain the stresses have reduced material dependence for any geometry of the inhomogeneity. The case when the outer boundary of the inhomogeneity annulus with eigenstrain is a free surface is also analyzed and agrees with classical surface tension results in the limit, but, moreover, the thick free surface terms (next order in the expansion depending on the radius) are also obtained and may induce instabilities depending on the bimaterial combinations. Applications of inhomogeneity annuluses with eigenstrain are wide and include interphases in thermal barrier coatings and coated particles in electrically/thermally conductive adhesives.

References:

X. Markenscoff and J. Dundurs, Annular Inhomogeneities with Eigenstrain and Interphase Modeling, *J.M.P.S.* http://dx.doi.org/10.1016/j.jmps.2013.12.003

On the Kinetics of Defect Motion

Rod Clifton, Professor of Engineering (Research), Brown University
Currently, Clark B. Millikan Visiting Professor of Aerospace, Cal Tech

Abstract

Consideration will be given to rate controlling mechanisms for dislocation glide in aluminum. At low stress levels the rate controlling mechanism is understood to be the thermally activated motion of dislocations past obstacles (e.g. forest dislocations and impurities). At high stress levels and elevated temperatures for which such obstacles are easily overcome, this defect motion is understood to be due to the intrinsic resistance of thermal phonons to the motion of dislocations. This transition in rate controlling mechanism has been investigated through molecular dynamics simulations, and through pressure-shear plate impact (PSPI) experiments on aluminum at high strain rates (10^6 s^{-1}) and at temperatures approaching melt. The molecular dynamics simulations, based on embedded atom potentials, have examined the effect of temperature on the mobility of dislocations in pure aluminum, and in Al-2.5%Mg and Al-5.0%Mg random substitutional alloys. The PSPI experiments have examined the high-strain-rate shearing resistance of high-purity aluminum over a range of temperatures where a transition in rate controlling mechanism from thermally activated motion to phonon drag can be expected. This talk will show preliminary indication of such a transition and raise questions for further study of the dependence of dislocation velocity on resolved shear stress and temperature at high dislocation velocities.

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A Unified Framework for Fracture and Plasticity

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Abstract

Plasticity and fracture share common features that have been recognized for some time. In both types of physical processes, the continuum is disrupted and the displacement field is no longer smooth across internal material surfaces. While significant effort has been devoted to the establishment of a computational framework to describe the motion and interaction of dislocation ensembles in materials (the Discrete Dislocation Dynamics - DDD-method), most recent computational efforts on fracture cast the problem within the framework of continuum elasticity. In this presentation, we lay the foundation for a unified description of both plasticity and fracture along the lines established for DDD; that is to model discontinuities explicitly. We first give and introduction and historical perspective, highlighting the pioneering works of Somigliana, Volterra and Burgers. Topological differences between cracks dislocations, and the associated stress fields are briefly discussed. We then present the Peierls-Nabarro model as a basis for describing the dislocation core, and extend its utility to the description of cracks. While the Peach-Koehler (PK) force is well-known in the field of dislocation mechanics, the Eshelby stress-momentum tensor will be presented as a basis for the PK force in plasticity, and equivalently for the J Integral in fracture. Motion of dislocations and the corresponding computational framework is derived from a variational principle and the principle of maximum entropy production, first introduced by Rayleigh and Onsager for general dissipative processes. Several examples of dislocation dynamics and crack mechanics will be presented.

“From Continuous to discrete dislocations”

Marcelo Epstein
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University of Calgary

Abstract

A unified theory of material defects, incorporating both the smooth and the singular descriptions, is presented based upon the theory of currents of Georges de Rham. The fundamental geometric entity of discourse is assumed to be represented by a single differential form or current, whose boundary is identified with the defect itself. The possibility of defining a less restrictive dislocation structure is explored in terms of a plausible weak formulation of the theorem of Frobenius. Several examples are presented and discussed.

A Geometric Formulation of the Nonlinear Mechanics of Distributed Defects

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Abstract: In this seminar we present a geometric framework in which the residual stress field of nonlinear solid can be analytically calculated. As examples, we consider solids with distributed line and point defects and distributed eigenstrains, and in particular, a nonlinear Eshelby's inclusion problem.

We first show that the nonlinear mechanics of solids with distributed dislocations can be formulated as a nonlinear elasticity problem provided that the material manifold – where the body is stress-free – is chosen appropriately. Choosing a Weitzenböck manifold (a manifold with a flat and metric-compatible affine connection that has torsion) with torsion tensor identified with the given dislocation density tensor the body would be stress-free in the material manifold by construction. We will present exact solutions for the residual stress field of several distributed dislocation problems in incompressible nonlinear elastic solids using Cartan's method of moving frames. We will also discuss zero-stress dislocation distributions in nonlinear dislocation mechanics.

We then calculate the residual stress field of a nonlinear elastic solid with a spherically-symmetric distribution of point defects. The material manifold is a flat Weyl manifold, i.e. a manifold with an affine connection that has non-metricity but both its torsion and curvature tensors vanish. Given a spherically-symmetric point defect distribution, we construct its Weyl material manifold using the method of Cartan's moving frames. In the case of arbitrary incompressible solids we calculate the residual stress field. We also compare the nonlinear and classical linear solutions.

This seminar is based on the following papers.

1. A. Yavari and A. Goriely, Riemann-Cartan geometry of nonlinear dislocation mechanics, *Archive for Rational Mechanics and Analysis* **205**(1), 2012, pp. 59–118.

2. A. Ozakin and A. Yavari, Affine development of closed curves in Weitzenböck manifolds and the Burgers vector of dislocation mechanics, *Mathematics and Mechanics of Solids*, 10.1177/1081286512463720.

3. A. Yavari and A. Goriely, Riemann-Cartan geometry of nonlinear disclination mechanics, *Mathematics and Mechanics of Solids* 18(1), 2013, pp. 91-102.

4. A. Yavari and A. Goriely, Weyl geometry and the nonlinear mechanics of distributed point defects, *Proceedings of the Royal Society A* **468**, 2012, pp. 3902-3922.

"F=FeFp? A kinematic analysis of finite elastoplasticity"

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William K. Gemmill Term Assistant Professor
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Sergio Conti
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Abstract

The kinematic description of finite elastoplasticity based on the decomposition F=FeFp is currently standard in the continuum mechanics community. Besides its acceptance, many issues have remained unresolved, such as the uniqueness of the decomposition, the characterization of the plastic deformation without reference to the intermediate configuration or its micromechanical understanding. In this talk, we will unveil some of these issues via a careful kinematic analysis of elastoplastic deformations at the microscale.

The Genetics of Size-Dependent Dislocation-Mediated Plasticity

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Size-affected dislocation mediated plasticity is important in a wide range of materials and technologies. Most existing predictive models are either empirically fitted laws that neglect the contribution of the microstructure, or merely account for it through ad-hoc assumptions. Here, a generalized size-dependent dislocation-based model that predict strength as a function of crystal/grain size and the dislocation density is developed. Three-dimensional discrete dislocation dynamics simulations reveal the first conclusive evidence of the existence of a well-defined relationship between strength and dislocation microstructure at all length scales for both single crystals and polycrystalline materials. The model predicts a transition from dislocation source strengthening to forest dominated strengthening occurs at a size-dependent critical dislocation density, which is directly proportional to the number of available dislocation sources in the crystal. It is also shown that the Hall-Petch relationship can be physically interpreted by coupling with the kinetic equation for the evolution of the dislocation density in polycrystals. The model is shown to be in remarkable agreement with experiments. This work provides a micro-mechanistic framework to predict and interpret strength size-scale effects and provides an avenue towards performing multiscale simulations without ad-hoc assumptions.

Anisotropic elasticity in dislocation dynamics

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The dislocation dynamics (DD) method models dislocations behavior, interactions and evolution in BCC and FCC materials. It is used to predict the strength of a material that varies with pressure, strain rate, temperature and evolving dislocation density by providing input parameters to continuum based approaches. Continuum models based on constitutive equations built using dislocation dynamics and molecular dynamics data have been successfully compared to high energy physics experiments in BCC tantalum and vanadium.

Large scale dislocation dynamics simulations usually involve several millions of interacting dislocation segments. The stress at a point and interaction force between two segments need to be computed many times during simulations. Up to now, DD simulations were restricted to isotropic elasticity calculations because using anisotropic elasticity was perceived as too expensive. We evaluate the cost versus accuracy of using spherical harmonics series to approximate the anisotropic elastic Green's function in calculating stresses and forces between segments. The stress at a point is obtained by analytically integrating the spherical harmonics series once and the forces by integrating it analytically twice. We analyze the convergence and cost of using this approach and describe the elements of a fast implementation.

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Singularity-free dislocation dynamics with strain gradient elasticity

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The singular nature of the elastic fields produced by dislocations presents conceptual challenges and computational difficulties in the implementation of discrete dislocation-based models of plasticity. In the context of classical elasticity, attempts to regularize the elastic fields of discrete dislocations encounter intrinsic difficulties. On the other hand, in gradient elasticity, the issue of singularity can be removed at the outset and smooth elastic fields of dislocations are available. In this work we consider theoretical and numerical aspects of the non-singular theory of discrete dislocation loops in gradient elasticity of Helmholtz type, with interest in its applications to three dimensional dislocation dynamics (DD) simulations. The gradient solution is developed and compared to its singular and non-singular counterparts in classical elasticity using the unified framework of eigenstrain theory. The fundamental equations of curved dislocation theory are given as non-singular line integrals suitable for numerical implementation using fast one-dimensional quadrature. These include expressions for the interaction energy between two dislocation loops and the line integral form of the generalized solid angle associated with dislocations having a spread core. The single characteristic length scale of Helmholtz elasticity is determined from independent molecular statics (MS) calculations. The gradient solution is implemented numerically within our variational formulation of DD, with several examples illustrating the viability of the non-singular solution. The displacement field around a dislocation loop is shown to be smooth, and the loop self-energy non-divergent, as expected from atomic configurations of crystalline materials. The loop nucleation energy barrier and its dependence on the applied shear stress are computed and shown to be in good agreement with atomistic calculations. DD simulations of Lomer-Cotrell junctions in Al show that the strength of the junction and its configuration are easily obtained, without ad-hoc regularization of the singular fields. Numerical convergence studies related to the implementation of the non-singular theory in DD are presented.

References:

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"Dynamic Discrete Dislocation Plasticity for the study of Plastic Relaxation under Shock Loading"

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ABSTRACT

Traditionally, the study of plastic relaxation processes under weak shock loading and high strain rates in metals has been based on direct experimental measurement of the macroscopic response of the material. Using this data, well-known macroscopic constitutive laws and equations of state have been formulated [1]. However, direct simulation of dislocations as the dynamic agents of plastic relaxation in those circumstances remains a challenge. Traditional methods of dislocation dynamics treat the elastic fields of dislocations quasistatically. That is to say, the explicit time dependence of the elastic fields is ignored; the force acting on a dislocation segment is calculated by evaluating the static stress fields of other dislocation segments in positions they occupy at a given instant in time. In this talk, it will be shown that when this approach is applied to shock loading, it violates causality: dislocations are activated ahead of the shock front. To avoid this artifact, a fully time-dependent formulation of the elastic fields for the creation and motion of dislocations must be introduced. Building on the pioneering work of Markenscoff and Clifton [2] we have showed in [3] how this can be done in 2D simulations, leading to a method we call "Dynamic Discrete Dislocation Plasticity" (D3P). In this talk, emphasis will be put on D3P's application to the study of inherently dynamic phenomena such as the elastic precursor decay under shock loading. Some relevant results in this respect will be presented and discussed.

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EXTREME DEFORMATION OF METALS BY PULSED LASERS

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The combination of high energy pulsed lasers, molecular dynamics computations, and characterization of recovered specimens is yielding an improved understanding on the fundamental deformation and failure mechanisms in metals. Our team has been pursuing these problems for fifteen years with the goal of elucidating these mechanisms. The following results will be discussed:

- Dislocations in shock compression: homogeneous generation vs. and multiplication.
- Void nucleation and growth: defects and kinetics.
- The slip twinning transition: material and external loading effects.
- The search for the elusive supersonic dislocation.

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Material strength and solid-state plasticity at high pressures and strain rates*

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Experiments are being done on high power lasers, such as the Omega laser at LLE and the Janus and NIF lasers at LLNL, to probe the solid-state plastic response of materials to high pressure (50-500 GPa), and very high strain rate deformation (1.e6 – 1.e10 1/s). Two classes of experiments will be described. Dynamic Laue diffraction experiments with a time resolution of ~0.1 ns have been developed to probe the microscopic lattice response of single crystal samples to a strong shock. In particular, the time scale for the onset of plasticity and the rate of the 1D to 3D lattice relaxation are a direct measure of how rapidly dislocations can be generated and transported on sub-nanosecond time scales (lattice kinetics). Macroscopic plastic flows at high pressure and strain rate can be generated that span a few tens of nanoseconds by using the Rayleigh-Taylor or Richtmyer-Meshkov fluid instabilities. Results from both classes of experiments will be compared with simulations using various models of flow stress (strength), a multi-scale model for bcc strength, and with analytic theory, where possible.

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