



International Center for Applied Computational Mechanics (ICACM)

Fifth Annual Symposium

The Role of Structure on Emerging Material Properties

Monday, June 11th to Wednesday, June 13th, 2012

Venue: The Kimmel Center at NYU
60 Washington Square South, 9th Floor (Room 912)



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Agenda

Session: Energetic Materials (June 11th, 2012)

Time	Title	Authors (affiliations)	Room
8:30 – 9:30 AM	-- REGISTRATION --	-- REGISTRATION --	KC912
9:30 – 9:40 AM	Opening Remarks	Dean Thomas Farris (Rutgers University)	KC912
9:40 – 10:20 AM	Atomic-Scale Theoretical Studies of Energy Transfer and Inelastic Deformation in Shocked PETN, RDX, and PBD	T. Sewell (University of Missouri)	KC912
10:20 – 11:00 AM	Experiments probing initiation and ignition of energetic materials	D. D. Dlott (University of Illinois Urbana Champaign)	KC912
11:00 - 11:15 AM	-- BREAK --	-- BREAK --	KC912
11:15 – 11:55 AM	Impact initiated Anaerobic reactions in powder mixtures: Instrumented Experiments and Meso-scale Simulations	N. Thadhani (Georgia Institute of Technology), Co-Authors: P. Specht, B. Aydelotte, J. Breidenich, M. Gonzales, D. Eakins	KC912
11:55 – 12:35 AM	Instabilities of planar detonation front in energetic materials	I. I. Oleynik (University of South Florida)	KC912
12:35 AM - 2:30 PM	-- LUNCH --	-- LUNCH --	LUPA's 170 Thompson Street, NY 10012
2:30 – 3:10 PM	Coarse grained simulations of high explosives	J.B. Maillet (DAM-CEA)	KC912
3:10 – 3:50 PM	Multi-scale modeling of solid propellants and energetic composites : challenges and advances	C. Nadot-Martin (Institut P'-DPMM) Co-Authors: D. Halm, A. Dragon, S. Dartois, A. Fanget	KC912
3:50 – 4:30PM	Response of a propellant under weak dynamics loading/ strategy and realizations	A. Fanget (CEA Gramat) Co-Authors: P. Mateille, G. Contesse, D. Jeulin, P. Lambert	KC912
4:30 – 4:40 PM	-- BREAK --	-- BREAK --	KC912
4:40 – 5:20 PM	Numerical simulations of a plastic bonded explosive submitted to low velocity impacts	D. Picart (CEA, DAM Le Ripault)	KC912
5:20 – 6:00 PM	Mesoscopic deformation and self-heating processes in a HMX-based PBX under a wide range of loading conditions	H. Trumel (CEA, DAM Le Ripault) Co-Authors: P. Lambert, M. Biessy, D. Picart, P. Bortoluzzi, A. Fanget	KC912



Session: Meta-Materials (June 12th, 2012)

Time	Title	Authors (affiliations)	Room
9:30 – 10:10 AM	Dynamic effective medium theory for periodic media	A. Norris (Rutgers University)	KC912
10:10 – 10:50 AM	A continuum theory of thermoelectric bodies and effective properties of thermoelectric composites	L. Liu (Rutgers University)	KC912
10:50 – 11:05 AM	-- BREAK --	-- BREAK --	KC912
11:05 – 11:45 AM	High contrast composites with unusual properties	G. Milton (University of Utah) Co-Authors: M. Briane, F.G. Vazquez, D. Onofrei, P. Seppecher, J. Willis	KC912
11:45 AM – 12:25 PM	Multiscale modelling of piezoelectric nanowires	J. Yvonnet (University of Paris) Co-Authors: M.T. Hoang, G. Chambaud, A. Mitrushchenkov	KC912
12:25 – 1:30 PM	-- LUNCH --	-- LUNCH --	KC912
1:30 – 2:10 PM	Fine-grained and ultrafine-grained FCC and HCP materials: microstructure and mechanical properties relationship under quasi-static and dynamic compression tests	G. Dirras (University of Paris) Co-Authors: H. Couque, G. Saada, P. Langlois	KC912
2:10 – 2:50 PM	Elastic models with intrinsic length for surface relaxation of diamond-like structures	A. Danescu (E. C. Lyon)	KC912
2:50 – 3:30 PM	A discontinuous-Galerkin formulation of Cohesive-Zone Models for the large-scale simulation of dynamic fracture and fragmentation	R. Radovitzky (Massachusetts Institute of Technology)	KC912
5:00 – 6:30 PM	-- POSTER and RECEPTION --	-- POSTER and RECEPTION --	KC912



Session: Coupled Phenomena (June 13th, 2012)

Time	Title	Authors (affiliations)	Room
9:00 – 9:40 AM	Molecular Basis for Nano-structure Property Relationships in Ni/Al Reactive Composites	A. Strachan (Purdue University) Co-Authors: M. J. Cherukara, K. GudaVishnu	KC912
9:40 – 10:20 AM	Insights into the Role of Structure on PBX Sensitivity	S. Bardenhagen (Wasatch Inc.) Co-Authors: J. Hooper, D. Bedrov, H. Luo, H. Lu, R. Armstrong, T. Harman	KC912
10:20 – 10:30 AM	-- BREAK --	-- BREAK --	KC912
10:30– 11:10 AM	Micro-poromechanics: recent advances in numerical models and perspectives	B. Chareyre (Grenoble)	KC912
11:10 – 11:50 AM	Degradation of granular media induced by internal fluid flow	L. Sibille (Nantes) Co-Authors: D. Marot, Y. Sail, P.Y. Hicher, F. Lominé, L. Scholtès	KC912
11:50 AM – 12:30 PM	Equivalent stress for multiphysics - Multiphysics couplings thanks to phase transformation description	O. Hubert (LMT – Cachan)	KC912



Abstracts

Session: Energetic Materials

Atomic-Scale Theoretical Studies of Energy Transfer and Inelastic Deformation in Shocked PETN, RDX, and PBD

Thomas D. Sewell, University of Missouri

Abstract: Theoretical studies of energy transfer in CHNO plastic-bonded explosive constituent materials will be discussed with an emphasis on the results and interpretation of medium- to large-scale molecular dynamics simulations of pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX), and polybutadiene (PBD) based on mechanically accurate but chemically non-reactive force fields. The focus will be on relatively weak shocks for which the principal interest is mechanical response rather than chemical reaction. Specific topics to be discussed include orientation dependent energy transfer and inelastic deformation subsequent to shock wave passage in initially defect-free PETN crystals, energy localization resulting from collapse of single and multiple voids in RDX crystals, and the dynamics of shock wave excitation and subsequent approach toward equilibrium in amorphous cis-PBD and at the RDX/PBD interface.

Experiments probing initiation and ignition of energetic materials

Dana D. Dlott, University of Illinois Urbana Champaign

Abstract: Two fundamental processes associated with shock compression of energetic materials (EM) are initiation and ignition. These processes can be quite different in molecular energetic materials and in reactive nanomaterials. In the chemical materials, initiation occurs just behind a shock front and ignition occurs anywhere from a few nanoseconds to hundreds of nanoseconds later. In reactive nanomaterials initiation may be the slower of the two processes. Experiments are described that probe the fundamental mechanisms of these processes on relevant length and time scales: picosecond vibrational spectroscopy of nanometer thick layers of energetic materials (EM) with laser-driven shock waves, and nanosecond emission spectroscopy of micrometer thick layers of EM using laser-driven flyer plates.

Impact initiated Anaerobic reactions in powder mixtures: Instrumented Experiments and Meso-scale Simulations

Naresh Thadhani, Georgia Institute of Technology

Co-Authors: P. Specht, B. Aydelotte, J. Breidenich, M. Gonzales, D. Eakins

Abstract: Impact initiation of reactions in various aluminum-based intermetallic-forming powder mixture compacts are being investigated using instrumented gas-gun impact experiments under conditions of uniaxial-strain and uniaxial-stress loading. Time-resolved stress and particle velocity measurements as well as high-speed imaging are used for monitoring the deformation and reaction states to obtain evidence of reaction based on changes in compressibility and shock-velocity, [1] as well as via direct light emission [2]. Meso-scale numerical simulations with CTH multimaterial hydrocode are also performed on actual (imported) micrographs [3]. The simulations allow qualitative and quantitative probing of the local configurational changes and their effects on impact-initiated reaction mechanisms, following validation of macroscopic properties by correlations with experiments. The heterogeneous nature of wave-propagation through reactants of dissimilar elastic and plastic properties and morphological characteristics, produce effects that give rise to turbulent flow, vortex formation, and dispersion of reactants across large distances. . Understanding of these processes as a function of mathematically represented constituent configuration and state of stress/strain is essential for designing energetic/reactive materials systems with



tunable energy release characteristics. This presentation will provide an overview of our experimental and modeling activities in understanding the mechanistic aspects of impact-initiation of reactions in various aluminum-based powder mixture compacts, relevant to the design of anaerobic reactive materials systems.

- [1] D. Eakins and N.N. Thadhani, "Discrete Particle Simulation of Shock Wave Propagation in a Binary Ni+Al Powder Mixture", *Journal of Applied Physics*, 2007, Vol. 101 (200) 043508-18.
- [2] E. Herbold, J.L. Jordan, N.N. Thadhani, "Observation of a minimum reaction initiation threshold in ball-milled Ni+Al under high-rate mechanical loading," *Journal of Applied Physics*, 109, 066108 (2011).
- [3] D.E. Eakins and N.N. Thadhani, "Mesoscale simulation of the configuration-dependent shock-compression response of Ni+Al powder mixtures," *Acta Materialia*, 56 (2008) pp. 1496-1510

Instabilities of planar detonation front in energetic materials

Ivan Oleynik, University of South Florida

Abstract: Detonation wave propagation in solid energetic materials (EMs), as described by the generic AB model, was investigated using a novel moving window molecular dynamics (MW-MD) technique. The atomic-scale simulations demonstrate that the detonation front is complex and becomes unstable by developing an inhomogeneous structure with low pressure and high pressure zones. Chemical reactions are initiated in local high-pressure Mach-stems with compressions and temperatures higher than those predicted by classical ZND theory. Transverse and longitudinal perturbations lead to a non-uniform energy release that makes the initially planar detonation front unstable. Different regimes of instabilities for a self-sustained detonation wave that result in cellular, oblique, spinning, or turbulent detonation fronts are discussed as a function of reaction barrier, sample size, and boundary conditions. These various instabilities of the planar detonation front in a solid AB EM, observed in MW-MD simulations, mirror the major regimes of gas-phase detonation, thus confirming the universal nature of detonation phenomena.

Coarse grained simulations of high explosives

Jean-Bernard Maillet, DAM-CEA

Abstract: We present recent developments of the Dissipative Particle Model that allow simulating the physico-chemical behavior of a molecular material at the mesoscale level. Structural and thermodynamic properties of the molecular crystal can be predicted qualitatively using an accurate intermolecular potential. We present simulations of the interaction of a shock wave with a defective crystal, and the subsequent hot spot behavior. Extension of this model that includes possible chemical reactions is presented, where additional degrees of freedom are attached to each mesoparticle.

Multi-scale modeling of solid propellants and energetic composites: challenges and advances

Carole Nadot-Martin, Institut P'-DPMM, France

Co-Authors: D. Halm, A. Dragon, S. Dartois, A. Fanget

Abstract: Solid propellants and energetic composites are made of energetic crystal particles randomly distributed in a soft elastomeric binder. The particle volume fraction is generally greater than 60% but is inferior to the corresponding fraction in high explosives such as Plastic-Bonded Explosives. Each phase exhibits a complex behavior that varies with loading conditions (temperature, strain rate, pressure) leading to a strongly non linear macroscopic response. Damage (particle cracking, interfacial debonding) complicates the overall response in addition to the complexities associated with the differing constitutive properties of the particles and binder phases. Regarding vulnerability, damage by grain/matrix debonding is an essential phenomenon to be tackled. First, interfacial defects are the privileged location for hotspots generation leading to the local initiation of a chemical reaction. Moreover, by increasing the specific surface offered to a flame, interfacial damage may drastically increase the propagation rate of combustion. These two events may trigger unexpected detonation even for moderate loading.



Scientific challenges underlying the multiscale modeling of solid propellants will be first presented as well as an overview of the existing tentative for both types of micromechanical approaches (micromechanics models, full-field simulations). Then, a non classical multiscale framework we developed for some ten years and attempted as an alternative to Eshelby inclusion-based micromechanics methods will be presented. The advanced approach results from a progressive research program aiming at estimating the non linear global response but also local fields and damage characteristics. The latest advances regarding finite strain viscoelasticity on one hand, and damage by interface debonding on the other hand, will be synthesized. Regarding the sound material, comparisons of estimates to reference solutions obtained by Finite Element full-field simulations, performed on real microstructures issued from X-ray tomography, will allow illustration of the modeling ability to account for challenges related to high volume fractions of particles and subsequent complex local interactions. Regarding damage, the homogenized and local responses of an artificial (i.e. numerically generated) microstructure, containing around 350 particles and submitted to a complex loading path, will be analyzed. Special attention will be paid to the evolution of the damage induced anisotropy as a function of the chronology of damage processes taking place at the microscale (nucleation/closure/re-opening of interfacial defects). The position and morphology of defects will be illustrated through 3D representations of the microstructure as well as the possible access to local field estimates with heterogeneity in the matrix depending on local morphology proper to the intergranular zone under consideration and on interfacial defects. As a result, the advanced modeling is able to capture complex interactions effects before and also during the failure process. As prospects, limits and future improvements of the multiscale model will be discussed.

Selected references:

Model without damage:

[1] C. Nadot-Martin, H. Trumel and A. Dragon, *European Journal of Mechanics A/Solids*, Vol. 22(1), pp. 89-106, (2003).

[2] C. Nadot-Martin, M. Touboul, A. Dragon and A. Fanget, Chapter 12 [in] *Multiscale Modeling of Heterogeneous Materials: From Microstructure to Macro-scale Properties*, O. Cazacu ed., ISTE/Wiley, pp. 218-237, (2008).

Model with damage:

[3] C. Nadot, A. Dragon, H. Trumel and A. Fanget, *Journal of Theoretical and Applied Mechanics*, Vol. 44(3), pp. 553-583, (2006).

[4] S. Dartois, C. Nadot-Martin, D. Halm, A. Dragon and A. Fanget, *Journal of Multiscale Modelling*, Imperial College Press, Vol. 1(384), pp. 347-368, (2009).

Response of a propellant under weak dynamics loading/ strategy and realizations

Alain Fanget, CEA Gramat

Co-Authors: P. Mateille, G. Contesse, D. Jeulin, P. Lambert

Abstract: One of the normative tests to improve safety of reactive material is the weight drop test apparatus. The analysis used to extract a safety response of the reactive material is makeshift. It can be summarized as a go no go test even if an energetic balance is done knowing the rebound of dropping mass. However, the scale of the description of the behaviour of a propellant is relative to its heterogeneities and the loading wavelength. The shorter it is, the more important the topological description of the material is. In our problems, involving the safety of energetic materials, the propellant can be submitted to a large spectrum of loadings. Starting from this normative test, we show several ways investigated to approach what going on to the material during the drop tests. The sample involved here is an ersatz of propellant composed of grains in a HTPB matrix. Firstly, we describe the changes done to the drop test apparatus in order to perform specific loading on the sample. In second are showed the developments realized to extract the morphology of the sample before and after the test in order to extract quantitative physical information. Thirdly, a numerical description at the mesoscale is suggested to try to simulated the loading path of the sample in the configuration of drop test. Finally, we list the lack of these investigations and give the future work.



Numerical simulations of a plastic bonded explosive submitted to low velocity impacts

Didier Picart, CEA, DAM Le Ripault

Abstract: The combustion to deflagration or detonation phenomenon in HMX-based pressed explosives is still poorly understood and as a result badly predicted today. Safety studies of pyrotechnic structures find thus benefit from a prediction of ignition conditions preliminary to any runaway of the reaction. We are interested here in the case of moderate mechanical impulses such as falls or impacts that do not directly lead to a shock-to-detonation transition.

Impact-induced pyrotechnic events are very complex phenomena, whose interpretation is hindered by difficulties coming from (1) the complexity of the dynamic loading, (2) the crucial role played by the non-linear behavior of the PBX, (3) the coupling of physical phenomena involving simultaneously deformation, self-heating, thermal conduction and chemical heat release and (4) the so-called but still unknown “hot-spot” process.

Therefore, any prediction of the full pyrotechnic event, including its violence, remains out of reach at present. We are only considering ignition rather than pyrotechnic reaction. This talk presents a numerical tool including our state of knowledge of the dynamic mechanical behavior of the PBX, the principles of the hot spot model development and a simplified heat equation. We evaluate the capabilities of the numerical tool for a large range of realistic impact scenario including drop-weight tests, Susan-tests, Steven-tests and a Taylor-test. The discussion highlights the relative good agreement between data and simulations as well as the future works that remain to be done.

Mesoscopic deformation and self-heating processes in a HMX-based PBX under a wide range of loading conditions

Hervé Trumel, CEA, DAM Le Ripault

Co-Authors: P. Lambert, M. Biessy, D. Picart, P. Bortoluzzi, A. Fanget

Abstract: Low velocity impacts ($<100 \text{ m}\cdot\text{s}^{-1}$) on HMX-based plastic-bonded explosives represent an important safety issue. In this case, ignition is known to proceed by hot spots processes, i.e. by small scale energy localization. The microstructure of the studied material appears as sub-millemetric HMX grains embedded in a composite matrix of much smaller HMX grains and a few percent rubbery binder, and bears a close resemblance with that of concrete. It behaves accordingly, displaying a strong sensitivity to stress triaxiality and, to a lesser extent, to strain rate. The dependence of deformation microprocesses to these two main loading parameters is studied by post-mortem optical microscopy on a series of samples recovered after various laboratory experiments. It is shown that microcracking and microplasticity are the main processes occurring at the scale of the microstructure. Their relative importance is essentially triggered by confining pressure. They are often associated with strong but very localized thermal effects, sometimes even observed after quasi-static loading. Recently, highly confined Hopkinson bar compression experiments were performed, allowing the combined effects of pressure and strain-rate to be studied. A mechanism close to adiabatic shear banding has been observed on some recovered samples, indicating that hot spots are not the only potential ignition mechanism. Up to now, the samples could only be recovered after 10-20% strain. Most ongoing efforts are dedicated to extending our strain capabilities to 50%, in order to approach the loading conditions undergone by the explosive during a real impact.



Session: Meta-Materials

Dynamic effective medium theory for periodic media

Andrew Norris, Rutgers University

Abstract: The concept of homogenized equations governing non-zero frequency behavior in periodic systems is discussed. Different effective equations can be obtained, depending on how the homogenization is defined. This non-uniqueness is illustrated with different homogenization schemes for a layered elastic medium. Most of the talk will describe a new method for dynamic homogenization of three-dimensional periodic elastic systems. The effective equations are of Willis form with coupling between momentum and stress. The fully dynamic effective material parameters govern the spatially averaged periodic part of the Bloch-Floquet solution. Numerical examples will be presented showing the variation of the parameters as a function of frequency. New issues arise in dealing with the wealth of information gained from the frequency dependence of the effective moduli. This suggests, among other things, that a better understanding of the frequency dependence might be achieved by not restricting consideration to the first Brillouin zone.

A continuum theory of thermoelectric bodies and effective properties of thermoelectric composites

Liping Liu, Rutgers University

Abstract: We develop a continuum theory for thermoelectric bodies following the framework of continuum mechanics and conforming to general principles of thermodynamics. For steady states, the governing equations for local fields are intrinsically nonlinear. However, under conditions of small variations of electrochemical potential, temperature and their gradients, the governing equations may be reduced to a linear elliptic system, which can be conveniently solved to determine behaviors of thermoelectric bodies. The linear theory is further applied to predict effective properties of thermoelectric composites. In particular, explicit formula of effective properties are obtained for simple microstructures of laminates and periodic E-inclusions, which implies useful design principles for engineering thermoelectric composites. We also discuss feasibility of large scale power generation by thermoelectric materials.

Metamaterials: high contrast composites with unusual properties

Graeme W. Milton, University of Utah

Co-Authors: M. Briane, F.G. Vasquez, D. Onofrei, P. Seppecher, J. Willis

Abstract: Composite materials can have properties unlike any found in nature, and in this case they are known as metamaterials. Recent attention has been focused on obtaining metamaterials which have an interesting dynamic behavior. Their effective mass density can be anisotropic, negative, or even complex. Even the eigenvectors of the effective mass density tensor can vary with frequency. Within the framework of linear elasticity, internal masses can cause the effective elasticity tensor to be frequency dependent, yet not contribute at all to the effective mass density at any frequency. One may use coordinate transformations of the elastodynamic equations to get novel unexpected behavior. A classical propagating wave can have a strange behavior in the new abstract coordinate system. However the problem becomes to find metamaterials which realize the behavior in the new coordinate system. This can be solved at a discrete level, by replacing the original elastic material with a network of masses and springs and then applying transformations to this network. The realization of the transformed network requires a new type of spring, which we call a torque spring. The forces at the end of the torque spring



are equal and opposite but not aligned with the line joining the spring ends. We show how torque springs can theoretically be realized.

Multiscale modelling of piezoelectric nanowires

Julien Yvonnet, University of Paris

Co-Authors: M.T. Hoang, G. Chambaud, A. Mitrushchenkov

Abstract: In this work, we propose a multiscale model of piezoelectric nanowires. The objective is to describe the overall size-dependent behavior of nanowires whose diameters range from a few nanometers up to millimeters. For that purpose, a continuum model is constructed, which incorporates additional surface energy arising from the free atoms on the surface at the nanoscale. Elastic and piezoelectric surface coefficients are characterized by ab initio calculations performed on slabs models. The proposed methodology allows separating surface and bulk energy contributions. To solve the continuum equations, a finite element framework taking into account the surface energy is described. Finally, to validate the continuum model, full ab initio solutions on nanowires models are solved and compared to the continuum solutions. Applications to AlN, ZnO and GaN nanowires are presented.

Fine-grained and ultrafine-grained FCC and HCP materials: microstructure and mechanical properties relationship under quasi-static and dynamic compression tests

Guy Dirras, University of Paris

Co-Authors: H. Couque, G. Saada, P. Langlois

Abstract: Various mechanical tests on nano-grained polycrystalline materials (NGP) have revealed a remarkable increase of strength, at the expense of ductility. However, the measured values of the yield stress of NGPs significantly differ from those obtained by extrapolating the Hall-Petch relationship. One reason for this discrepancy lies in an inaccurate description of the elastic-plastic transition. Indeed, due to the processing conditions, and to the grain size, both the macroyield stress and the macroyield strain of NGPs differ from those of coarse-grained polycrystals (CGP). Despite the large amount of papers published in the last decade on the subject, a comprehensive description of the deformation, damage and strengthening mechanisms of these materials is still lacking. Indeed, our present understanding of the deformation mechanisms of conventional CGPs depends on: (i) processing specimens with well designed and characterized microstructures; (ii) gathering consistent and systematic data through mechanical tests over a wide range of strain rates and in a large temperature interval; (iii) thoroughly observing the evolution of the microstructure during mechanical testing; and (iv) establishing a consistent correlation of the mechanical behavior with the microstructure by a relevant theoretical analysis. Instead, for NGPs, the present situation is characterized by: (i) unsatisfactory control and description of the as-prepared microstructure; (ii) incomplete information on the evolution of the microstructure; (iii) inaccuracy of the measurement of the relevant mechanical parameters; (iv) inadequate theoretical interpretation: in the case of CGPs, there is a general, and justified agreement on the relevance of the identification of the 0.2% proof strain flow stress $\sigma_{0.2}$ to the yield stress σ_Y . The extension of these assertions to the case of NGPs is questionable. After a brief review of the state-of-the-art, this lecture will focus on microstructure-mechanical properties relationship of fine-grained and ultrafine-grained metallic materials processed by different routes and submitted to quasi-static and/or dynamic compression tests at room temperature. Multi-scale microstructure engineering for ductility enhancement will be presented and discussed.

Elastic models with intrinsic length for surface relaxation of diamond-like structures

Alexandre Danescu, E. C. Lyon

Abstract: Motivated by experimental evidence for ultra-small structures, we overview the minimal ingredients needed to describe both bulk and surface effects in nano-structured materials. Starting from the valence force field model we construct two models with intrinsic length: the first one follows the line of



successive polynomial approximations in the first Brillouin zone while the second one is based on the notion of geometrical incompatibilities in the discrete setting. From available experimental data we determine all material parameters for both models and discuss their ability to predict size and shape effects. Special attention is devoted to average lattice parameter variations in nano-porous silicon.

A discontinuous-Galerkin formulation of Cohesive-Zone Models for the large-scale simulation of dynamic fracture and fragmentation

Raul Radovitzky, Massachusetts Institute of Technology

Abstract: Understanding the fracture and fragmentation of brittle solids under impact loading remains one of the most difficult challenges in solid mechanics. As a specific example of practical interest, brittle plates subject to localized impact loads exhibit intricate patterns of fracture and fragmentation which include radial, conical and lateral cracks. The accurate description of the formation and evolution of these features is fundamental for understanding and assessing the ballistic performance of ceramic armor, especially in multi-hit scenarios.

In this presentation, I will describe an algorithm for the scalable simulation of fracture and fragmentation in brittle materials. The method is based on a combination of a discontinuous Galerkin (DG) formulation of the continuum problem and Cohesive Zone Models (CZM) of fracture. Prior to fracture, the flux and stabilization terms arising from the DG formulation at interelement boundaries are enforced via interface elements, much like in the conventional intrinsic cohesive element approach, albeit in a way that guarantees consistency and stability. This eliminates wave propagation issues typical of intrinsic cohesive element approaches. Upon the onset of fracture, the traction-separation law (TSL) governing the fracture process becomes operative without the need to insert a new cohesive element. Upon crack closure, the reinstatement of the DG terms guarantee the proper description of compressive waves across closed crack surfaces.

A key feature of the method is that it avoids the need to propagate topological changes in the mesh as cracks and fragments develop, which enables the indistinctive treatment of crack propagation across processor boundaries and, thus, the scalability in parallel computations. The scalability of the proposed DG/CZM method is demonstrated on up to 4096 processors and problems of up to 3.1 billion degrees of freedom.

As an example of the versatility of the method, we demonstrate its ability to capture intricate patterns of radial and conical cracks arising in the impact of ceramic plates.

Session: Coupled Phenomena

Molecular Basis for Nano-structure Property Relationships in Ni/Al Reactive Composites

Alejandro Strachan, Purdue University

Co-Authors: M. J. Cherukara, K. GudaVishnu

Abstract: Intermolecular Reactive Composites have generated significant interest in fields as diverse as defense, microelectronics and medicine due to their high exothermicity and fast reaction rates, tunable properties, and the potential for multi-functionality. However, the mechanisms that govern the initiation



and propagation of the reaction are poorly understood and, thus, relationships between nano- and microstructure and properties are not firmly established. This lack of fundamental knowledge has hindered their optimization and application. We use molecular dynamics to simulate the exothermic reaction of Ni/Al nano-laminates at different temperatures, periodic lengths and nanostructures. We show that the reaction is diffusion controlled in the bulk phase but the introduction of defects like porosity or a free surface speed up the reaction rates enormously. Furthermore, the relationship between reaction timescales and nanostructure change as ballistic transport mechanisms are enabled by the extended defects.

We use molecular dynamics simulations to explore the potential use of amorphous metals in intermolecular reactive composites. Our simulations show that amorphous Ni/Al nano-laminates lead to an increase in temperature of up to 260 K over their crystalline counterparts, this increase corresponds to over 20% of the heat of fusion and can be explained in terms of the amorphization energy. These results indicate that amorphous metals are attractive candidates for energetic formulations.

Insights into the Role of Structure on PBX Sensitivity

Scott Bardenhagen, Wasatch Inc.

Co-Authors: J. Hooper, D. Bedrov, H. Luo, H. Lu, R. Armstrong, T. Harman

Abstract: Plastic-Bonded Explosives (PBXs) are composed of energetic grains embedded in a polymeric binder. Heterogeneity at this material scale serves to localize energy during deformation, resulting in a broad spectrum of conditions at the mesoscale, the scale of the grains. This localization determines material damage, hot spot development and, ultimately, sensitivity. Here an overview of a combined experimental and modeling effort, focused on the role of mesoscale structure in the response of PBXs in highly confined environments, is presented. A suite of mock materials was carefully prepared to vary mesoscale characteristics such as binder loading and grain size distribution. These materials, along with the individual constituents, generated a continuum of material response over a wide range of conditions. The “controlling” role of the binder was convincingly demonstrated, and, in particular, the importance of its pressure dependent response. Confinement leads to glassy binder material properties, which in turn promotes highly localized plasticity in the grains, potentially resulting in hot spots and fracture. This mechanism may be particularly important in confined conditions relative to other, generally more commonly considered, hot spot mechanisms. It also appears to be enhanced by an embrittling effect of the plasticizer, which was also investigated in detail. PBX mesoscale structure was extensively investigated for the material suite. Xray microtomography was used to determine three-dimensional morphologies. Specialized image processing routines were used to identify individual features (voids, grains, binder) for numerical discretization. The quantity of material needed to accurately represent the mesoscale structure in simulations, i.e. the representative volume element size, was determined. Additional mesoscale structure characteristics were also identified in these analyses, including grain on grain contact density, which is expected to correlate with material sensitivity, particularly on account of hot spots due to highly localized plasticity in the grains. Results from mesoscale structure analyses, as well as from computations using these mesoscale structures, will be reported with a focus on implications for PBX sensitivity under confined conditions.

Micro-poromechanics: recent advances in numerical models and perspectives

Bruno Chareyre, Grenoble

Abstract: The numerical models of granular materials have been developed and used for decades now, and provide invaluable tools for micromechanical studies of geomaterials. The coupling of these models with pore fluids started more recently. It is currently the object of very active developments, and it has many potential applications. The different kinds of coupling methods are reviewed and discussed. Our latest developments on the modeling of capillary effects and seepage flow are presented. It is shown that the formulation of a flow problem at the pores scale result in a discrete form of the classical equations of poromechanics, with the constitutive behaviour linked directly to some micro-scale properties of the



granular assembly. Results concerning the complex interaction between near-shore waves and seabed sediments are presented. Finally the next challenges for numerical models are discussed.

Degradation of granular media induced by internal fluid flow

Luc Sibelle, Nantes

Co-Authors: D. Marot, Y. Sail, P.Y. Hicher, F. Lominé, L. Scholtès

Abstract: The mechanical behaviour of saturated granular media is classically investigated independently of a hydraulic loading generated, on the granular skeleton, by an internal fluid flow. On the other side, hydraulic properties of granular media is also commonly characterized independently of a possible evolution of their microstructures. However, interactions between the interstitial fluid flow and the solid granular skeleton can be particularly complex and requires a fully coupled description. Granular skeleton can be partially destructured by an internal flow leading to a degradation of its load bearing capacity; fluid flow and thus the hydraulic loading may be affected by particle rearrangements induced either by the strain response of the granular assembly to an external mechanical loading, or by the seepage flow itself. A challenging point today is to describe these complex interactive behaviours involved, for instance, in the durability of soil buildings as dams or dykes, in soil slope stability, or in foundation bearing capacity.

In this context, we present first experiments performed on glass bead assemblies to illustrate the different aspects of such solid-fluid interactions. Then an overview of different approaches, from uncoupled models to fully coupled ones, to tackle one or several sides of the problem is presented. Complementarity and exchange of information between these different approaches should lead to a complete description (currently missing) of such coupled phenomena, from the action of the fluid flow on the stressed granular skeleton, to the response, at a large scale, of the structure in terms of deformation and failure.

Equivalent stress for multiphysics - Multiphysic couplings thanks to phase transformation

Olivier Hubert, LMT - Cachan

Abstract: Materials and structures exhibiting coupled behaviors between mechanics and other physics (especially magnetics, electrics and thermics – phase transformation –) and submitted to multiaxial stress are considered. The most practical applications concern sensors and actuators. The multiaxial stress is usually inherited from forming process or appears in use. In the area of coupling between mechanics and magnetics, one can mention inertial stresses in high rotating speed systems or new technologies of flywheel, stresses due to binding process (encapsulation), residual stress associated to plastic straining (forming) or cutting process. On the other hand, since the works of Mateucci [1] and Villari [2], mechanical stress is known to change significantly the magnetic behavior of materials (see for instance [3]) as well as their magnetostrictive behavior [4]. The design of electromagnetic systems consequently requires coupled models taking account of multiaxial stress. One way is to use energy-based models written at an appropriate scale. Indeed the development of fully multiaxial magneto-elastic models following micromagnetics is a promising issue [5–7], but still leads to dissuasive computation times for engineering design applications. The few available and practically implemented models describing the effect of stress on the magnetic behavior are restricted to uniaxial (tensile or compressive) stress. Jiles–Atherton type models [8–9] and Preisach type models [10–11] are the most popular. Indeed the relevant way seems to implement multiaxial stress directly in a uniaxial model. This way supposes to define and calculate a “fictive” uniaxial stress, the equivalent stress that would change the magnetic behavior in a similar manner than the multiaxial one. Such equivalent stress has been proposed recently [12]. It is based on equivalence in magnetization and uses an analytical discretization of bulk in so-called magnetic domains. The free energy of each domain is written allowing calculate their volume fraction thanks to a stochastic approach (calculation thanks to Boltzmann function). Macroscopic magnetization is the average magnetization over the volume. Since an equilibrium of phases is involved, the approach proposed for magneto-elastic coupling can be extended to ferroelectric media, and other couplings where a form of phase transformation occurs. Application to the modeling of thermo-mechanical behavior of shape



memory alloys is finally made. The talk will be illustrated by experimental results carried out on magnetic materials and shape memory alloys submitted to uniaxial and multiaxial stresses.

KEYWORDS: multiphysic couplings, magneto-elasticity, electro-elasticity, phase transformation, equivalent stress.

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Directions and Maps

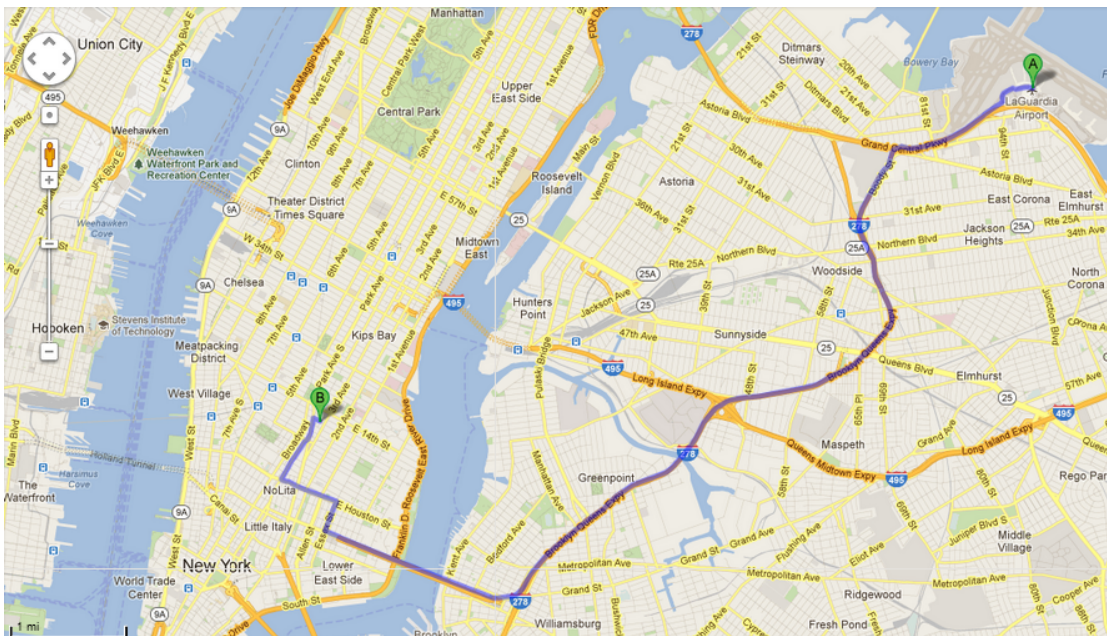
Driving from LaGuardia Airport, New York to Founders Hall

From: LaGuardia Airport (LGA)

1. Head northwest on LaGuardia Rd toward 94th St 0.3 mi
2. Slight left onto 94th St 249 ft
3. Take the ramp onto Grand Central Pkwy 0.8 mi
4. Take exit 4 for Brooklyn-Queens Expressway toward Interstate 278 W/Staten Island 0.2 mi
5. Merge onto Brooklyn Queens Expy E 1.0 mi
6. Merge onto I-278 W 4.6 mi
7. Take exit 32A on the left toward Williamsburg Bridge/Manhattan 0.5 mi
8. Merge onto Williamsburg Bridge 1.5 mi
9. Turn right onto Essex St 0.3 mi
10. Turn left onto E Houston St 0.5 mi
11. Turn right onto Lafayette St 0.5 mi
12. Continue onto 4th Ave 0.1 mi
13. Turn right onto E 12th St, Destination will be on the right 348 ft

To: Founders Hall

120 E 12th St, New York, NY 10003





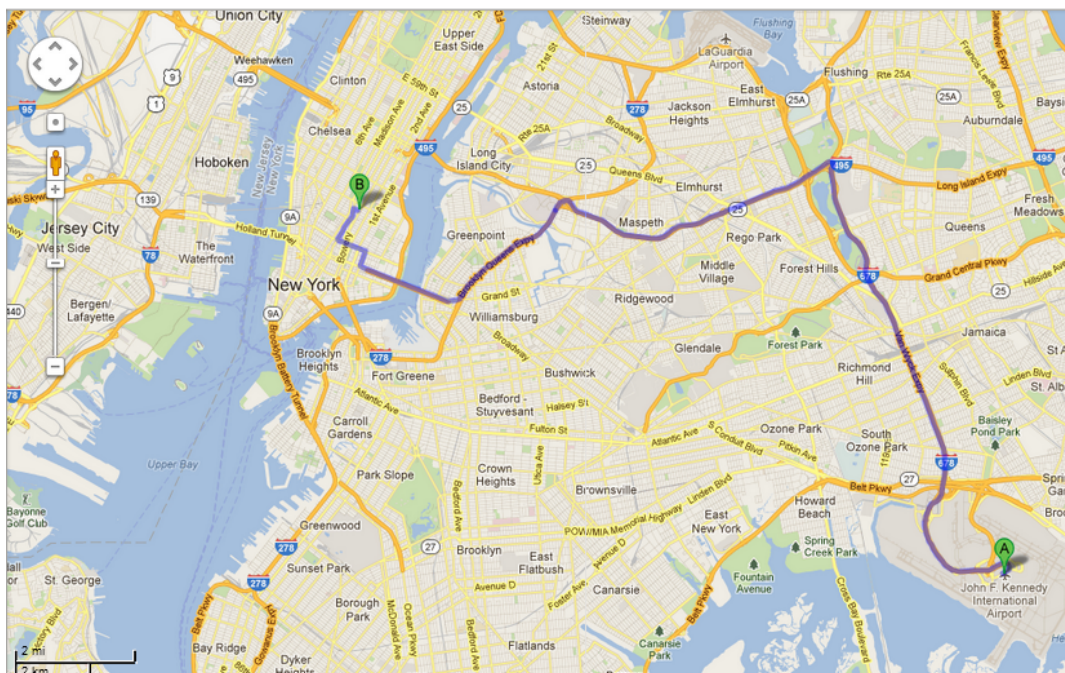
Driving from John F. Kennedy Airport, New York to Founders Hall

From: John F. Kennedy Airport (JFK)

- | | |
|--|--------|
| 1. Head northeast | 0.2 mi |
| 2. Take the ramp to Airport Exit | 266 ft |
| 3. Merge onto JFK Access Rd | 0.2 mi |
| 4. Continue onto Van Wyck Expy | 0.7 mi |
| 5. Continue onto I-678 N | 7.4 mi |
| 6. Take exit 12B for I-495 W/L I Expy toward Midtown Tun | 0.5 mi |
| 7. Merge onto I-495 W | 3.4 mi |
| 8. Take exit 17W toward Brooklyn | 1.4 mi |
| 9. Merge onto I-278 W | 2.0 mi |
| 10. Take exit 32A on the left toward Williamsburg Bridge/Manhattan | 0.5 mi |
| 11. Merge onto Williamsburg Bridge | 1.5 mi |
| 12. Turn right onto Essex St | 0.3 mi |
| 13. Turn left onto E Houston St | 0.5 mi |
| 14. Turn right onto Lafayette St | 0.5 mi |
| 15. Continue onto 4th Ave | 0.1 mi |
| 16. Turn right onto E 12th St, Destination will be on the right | 348 ft |

To: Founders Hall

120 E 12th St, New York, NY 10003





Walking from Founders Hall to Kimmel Center

From: Founders Hall

120 E 12th St, New York, NY 10003

1. Head northwest on E 12th St toward 4th Ave
2. Turn left onto University Pl
3. Continue straight onto Washington Square E
4. Turn right onto Washington Square S, Destination will be on the left

0.2 mi

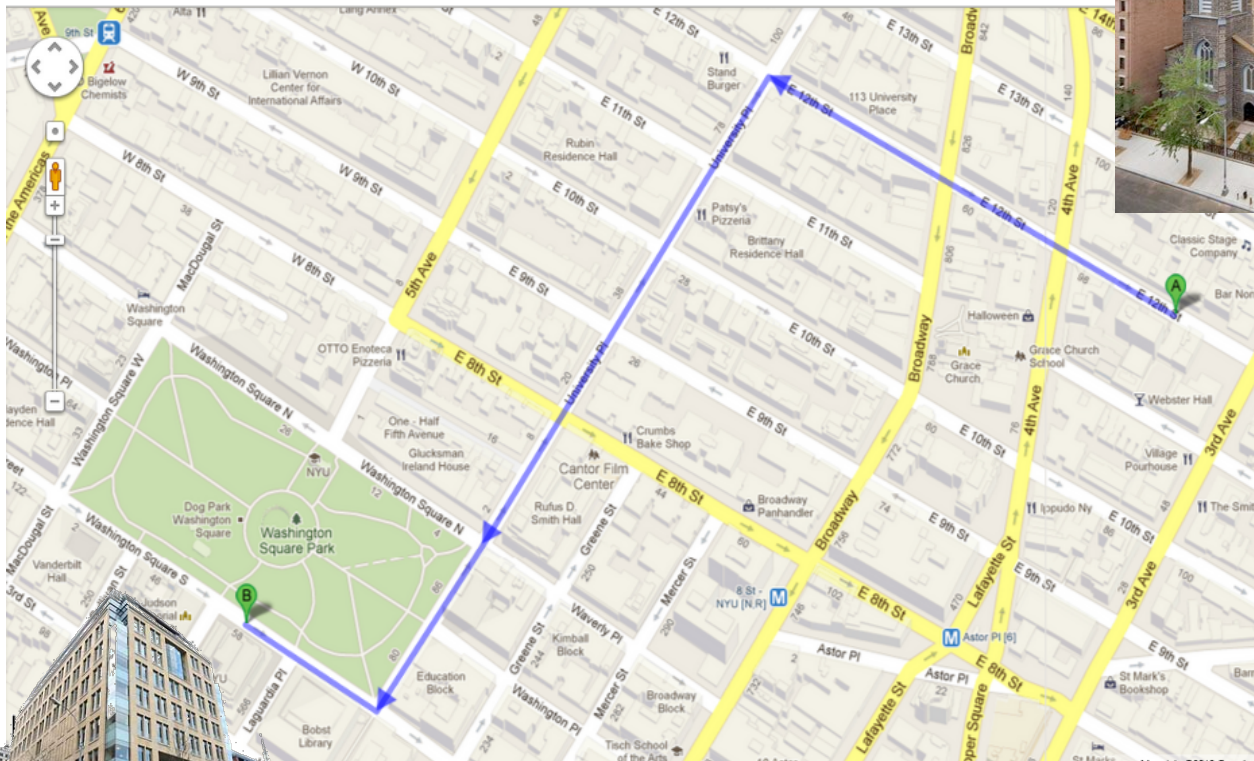
0.3 mi

499 ft

410 ft

To: NYU Kimmel Center for University Life

60 Washington Square South, New York, NY 10012



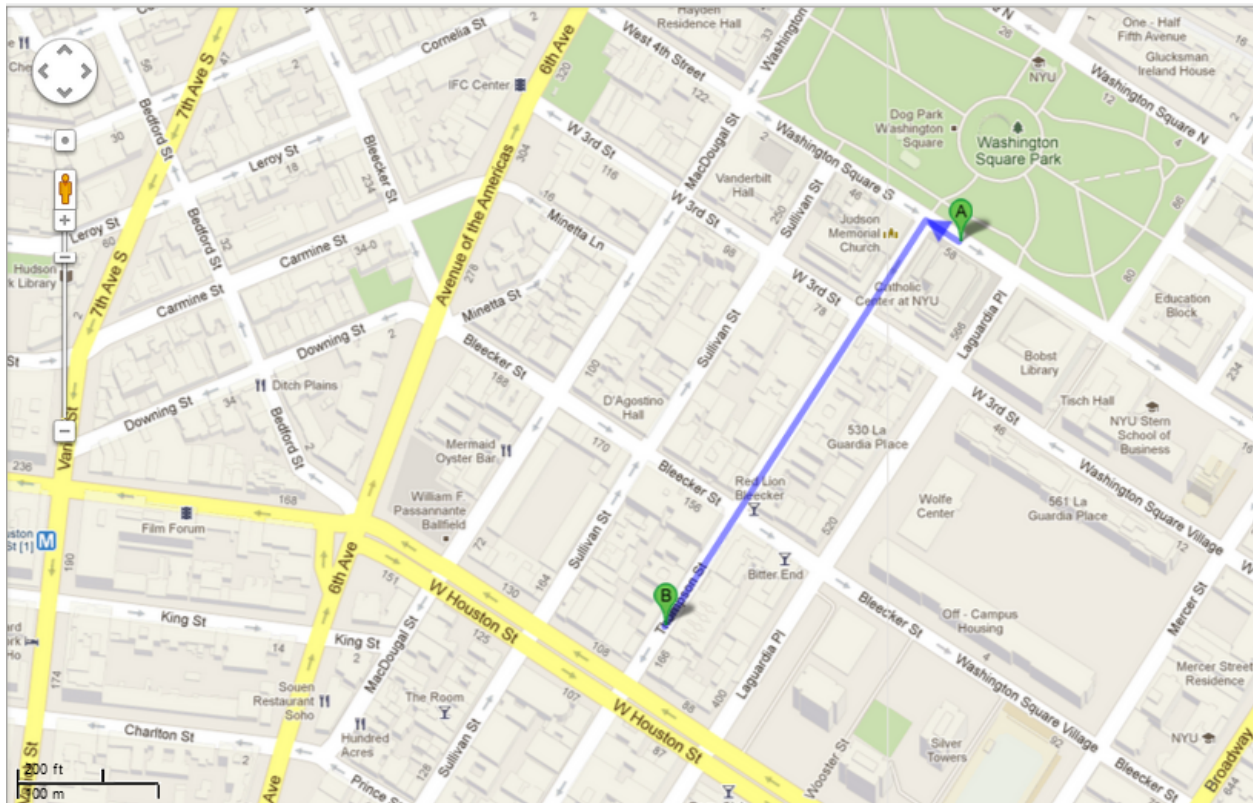


Walking from Kimmel Center to Lupa Restaurant

From: NYU Kimmel Center for University Life
60 Washington Square South, New York, NY 10012

1. Head northwest on Washington Square S toward Thompson St 92 ft
2. Turn left onto Thompson St 0.2 mi

To: Lupa Osteria Romana
170 Thompson Street, New York, NY 10012





Directions to Kimmel Center

By Subway

- Take the A, C, E, B, D, F, M trains to **West 4 Street-Washington Square**, and walk east on West 4 Street for about 4 blocks.
- Take the N, R trains to **8 Street-NYU**, walk south on Broadway to West 4 Street and then walk westward.
- Take the 6 train to **Astor Place**, and go west on Astor Place to Broadway. Walk south on Broadway to West 4 Street and then walk westward.

By Plane

- From **La Guardia Airport**:
take the Q33 bus to **74 Street Bus Terminal**, and transfer for a **Manhattan-bound F** train; or take the M60 bus to **Hoyt Avenue/31 Street**, and transfer for a **Manhattan-bound N** train. (see subway instructions above)
- From **JFK Airport**:
take the AirTrain to **Howard Beach**, and transfer for a **Manhattan-bound A** train. (see subway instructions above)
- From **Newark Airport**:
take NJ Transit trains or the airport shuttle bus to **New York Penn Station** or **Port Authority Bus Terminal**, and take **Brooklyn-bound A, C, E** trains; or to **Grand Central**, and take a **Brooklyn-bound 6** train. (see subway instructions above)

Cabs and car services are available at the airport with variable cost depending on the airport and time of day.

By Train

- Take PATH train to **9 Street**, and walk south on 6 Avenue to West 4 Street and then walk east for about 4 blocks.
- Take LIRR, Amtrak, NJ Transit trains to **New York Penn Station**, and take **Brooklyn-bound A, C, E** trains. (see subway instructions above)
- Take Metro-North train to **Grand Central Station**, and take a **Brooklyn-bound 6** train. (see subway instructions above)

By Car

- **From Connecticut, the Bronx and Upstate NY**
Take the I-95/I-278, or NY State Thruway (Major Deegan Expressway in the Bronx) to RFK Bridge (toll). Cross to Manhattan taking the FDR Drive south to Houston Street. Continue west on Houston Street past Broadway to La Guardia Place. Turn right and proceed until Washington Square.



- **From the Northwest, West, and South including New Jersey**
Take the I-95 and/or the New Jersey Turnpike to Lincoln Tunnel or Holland Tunnel. If taking the Lincoln tunnel, make a left turn on to 34 Street, and turn left onto 9 Avenue after one block. Then proceed to south until 14 Street. Turn left onto 14th Street followed by a right onto 5 Avenue to Washington Square. If taking the Holland tunnel, there will be a circle after exiting. Take the Canal Street east to West Broadway. Turn left and proceed until you reach Washington Square.
- **From the George Washington Bridge**
Take the Henry Hudson Parkway (turns into the West Side Highway/12 Avenue) south to 23 Street. Turn left on 23 Street to 5 Avenue. Turn right on 5 Avenue to Washington Square.
- **From Brooklyn, Staten Island**
Take the Verrazano-Narrows Bridge/Belt Parkway west to the Brooklyn-Queens Expressway (BQE) east. Take the Manhattan Bridge exit, cross over the bridge, take Canal Street west to 6 Avenue, turn right and travel north to West 4 Street and travel east.
- **From Long Island, Queens**
Take the Long Island Expressway (I-495) west to the Queens-Midtown Tunnel. Drive west on 37 Street to 5 Avenue. Turn left on 5 Avenue to Washington Square.