

# WHY IS STABILITY IMPORTANT IN SOLIDS?

IN DESIGN WE GENERALLY ADDRESS TWO ISSUES:

- CHECK OPERATING LOADS (STRESSES WITHIN ELASTIC LIMITS)
- **DESIGN TO AVOID FAILURE (SAFETY AT EXTREME LOADS)**

FAILURE OF STRUCTURES FALLS INTO TWO BASIC TYPES:

- FRACTURE (STRESS CONCENTRATION AT LOCAL FLAWS)
- **BUCKLING (OVERALL STRUCTURAL FAILURE DUE TO INSTABILITY)**

**REASON** FOR BUCKLING INSTABILITY: **NONLINEAR** BEHAVIOR OF STRUCTURES

STUDY OF STABILITY IMPORTANT NOT ONLY FOR ENGINEERING STRUCTURES, BUT FOR A MUCH WIDER RANGE OF APPLICATIONS IN SOLIDS AND MATERIALS



### **COURSE OVERVIEW**

- 1. Concept of stability and examples of discrete systems
- 2. Concept of bifurcation and examples of discrete, conservative systems
- 3. LSK asymptotics for perfect continua & 1D application (elastica) simple mode case
- 4. 2D application (plate) & LSK asymptotics for imperfect continua simple mode case
- 5. LSK asymptotics for perfect continua & 2D application (plate) multiple mode case
- 6. FEM techniques for continuum elastic systems. Buckling of fiber-reinforced composites
- 7. Stability of honeycomb under compressive loading Bloch wave representation
- 8. Phase transformations in shape memory alloys: continuum & 3D lattice models
- 9. Review



### **NEW CONCEPTS INTRODUCED**

- 1. Concept of stability (here of an equilibrium)
  - 1. Linearization method
  - 2. Lyapunov's direct method
- 2. Concept of **bifurcation** (here for equilibria of **conservative**, elastic systems)
  - 1. Limit point vs bifurcation point
  - 2. Imperfections change bifurcation to limit points (or lower singularity order)
  - 3. Imperfections: amplitude vs shape
- 3. LSK asymptotics for continuum conservative systems : reduce study of an infinite problem to the study of a finite-dimensional one near the critical point.



## **STABILITY OF EQUILIBRIUM STATES**

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### TWO WIDELY USED METHODS TO CHECK STABILITY:

#### 1. LINEARIZATION METHOD

- a) Linearization of the equations of motion about equilibrium state
- b) Stability analysis of the linearized perturbed motions

**STABILITY** if all eigenvalues have non-positive real part

c) Justification of the results with respect to the actual motion of the system

#### 2. LYAPUNOV'S DIRECT METHOD

**STABILITY** guaranteed when a non-increasing functional L(p(t)) can be found that satisfies certain bounding properties for the initial conditions and the current state



### LINEARIZATION METHOD

 $\dot{\mathbf{p}} = \mathbf{f}(\mathbf{p}) = \mathbf{f}(\mathbf{p}_e) + \left[\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\right]_e [\mathbf{p} - \mathbf{p}_e, ] + \mathbf{o}(\|\mathbf{p} - \mathbf{p}_e\|), \text{ Taylor series expansion of } \mathbf{f}$ 

 $0 = \mathbf{f}(\mathbf{p}_e),$  recall from equilibrium

 $\Delta \mathbf{p} \equiv \mathbf{p} - \mathbf{p}_e, \quad \mathbf{A} \equiv \left[\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\right]_e, \quad \text{definitions}$ 

 $\Delta \dot{\mathbf{p}} = \mathbf{A} \Delta \mathbf{p}$ , LINEARIZED SYSTEM (approximates actual one)

 $\Delta \mathbf{p}(t) = \exp[t\mathbf{A}]\Delta \mathbf{p}(0), \text{ solution of linearized system}$   $\Delta \mathbf{p}(t) \text{ bounded } \forall t > 0 \text{ iff } \Re(a_i) < 0 \forall \text{ eigenvalues } a_i \text{ of } \mathbf{A}$  **STABILITY OF LINEARIZED SYSTEM** 

**NOTE** : for simplicity  $\partial \mathbf{f} / \partial t = 0$ , autonomous system  $\implies \mathbf{A}$  is a constant matrix



### LINEARIZATION METHOD (LYAPUNOV'S THEOREM)

- If the real part of all the eigenvalues a<sub>i</sub> of the linearized system's matrix A are negative, (not necessarily strictly so) the system is stable
  - If the real part of at least one eigenvalue a<sub>i</sub> of the linearized system's matrix A is strictly positive, the system is unstable

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**NOTE:** Proof of stability for nonlinear system requires additional information about the growth of the difference between the linearized and nonlinear systems



### LYAPUNOV'S DIRECT METHOD

A system is stable if a functional L(p(t)) can be found with the following properties:

- $\frac{dL}{dt} \leq 0$ , (functional is nonincreasing)
- $L(\mathbf{p}(t)) \ge c \parallel \mathbf{p}(t) \mathbf{p}_e \parallel^2, \ (c > 0; \text{ functional measures distance from equilibrium})$
- $L(\mathbf{p}(0)) \leq d \parallel \mathbf{p}(0) \mathbf{p}_e \parallel^2, \ (d > 0; \text{ functional measures initial perturbation})$

#### **PROOF** :

 $c \parallel \mathbf{p}(t) - \mathbf{p}_e \parallel^2 \leq L(\mathbf{p}(t)) \leq L(\mathbf{p}(0)) \leq d \parallel \mathbf{p}(0) - \mathbf{p}_e \parallel^2 \Longrightarrow \parallel \mathbf{p}(t) - \mathbf{p}_e \parallel \leq \varepsilon; \ (\eta \leq \varepsilon \sqrt{c/d})$ 

**NOTE**: Finding a Lyapunov functional for a stable system is **not always** possible

CONSERVATIVE SYSTEM IS **STABLE** IFF POTENTIAL ENERGY **MINIMIZED** AT EQUILIBRIUM



### BIFURCATION OF EQUILIBRIUM SOLUTIONS IN CONSERVATIVE, NONLINEAR SYSTEMS

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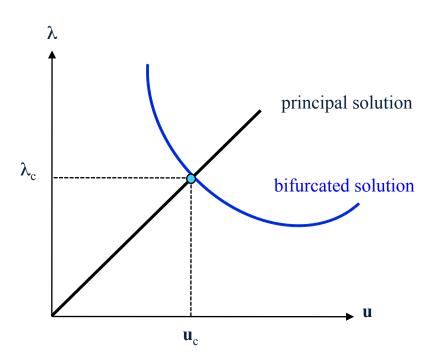
#### FUNDAMENTAL ASSUMPTIONS USED:

- Systems are time-independent
- Systems are conservative, i.e. they have an energy which remains constant
- Energy depends on a scalar parameter  $\lambda$  (termed load parameter)

• Systems are nonlinear, i.e. energy is non-quadratic function of independent variable and as a result for a given  $\lambda$ , multiple equilibrium solutions can be found

• Stability of these equilibrium solutions are examined by investigating if their energy has a local minimum at these solutions





**BIFURCATION:** Loss of uniqueness – as a function of a control parameter – in the solution of a nonlinear system of equations. Bifurcated branch typically emerges as a "fork" from the principal branch.

- System:  $f(u,\lambda) = 0$
- Principal solution starts at  $\lambda = 0$ ,  $\mathbf{u} = \mathbf{0}$
- Bifurcated solution emerges from principal one at the critical point  $\lambda_c$

 $\mathcal{E}(\mathbf{u}, \lambda)$ : energy of system at displacement  $\mathbf{u} \in \mathbb{R}^n$  and load  $\lambda \ge 0$ 

 $\mathbf{f}(\mathbf{u}, \lambda) \equiv \mathcal{E}_{,\mathbf{u}} = \mathbf{0}, \quad \text{equilibrium is energy extremum}: \ \mathcal{E}_{,\mathbf{u}} \equiv \partial \mathcal{E} / \partial \mathbf{u}$ 

$$\overset{0}{\mathbf{u}}(\lambda)$$
: principal solution i.e.  $\mathbf{f}(\overset{0}{\mathbf{u}}(\lambda),\lambda) = \mathbf{0}, \ \forall \lambda \ge 0; \ \overset{0}{\mathbf{u}}(0) = 0$ 

 $\mathcal{E}_{,\mathbf{u}\mathbf{u}}\Delta\mathbf{u} + \mathcal{E}_{,\mathbf{u}\lambda}\Delta\lambda \approx \mathbf{0} \implies \Delta\mathbf{u} \approx -\Delta\lambda[\mathcal{E}_{,\mathbf{u}\mathbf{u}}]^{-1}[\mathcal{E}_{,\mathbf{u}\lambda}]; \text{ construct } \overset{0}{\mathbf{u}}(\lambda) \text{ by continuation}$ 



$$\mathcal{E}^{c}_{,\mathbf{u}\mathbf{u}} \equiv \left[\frac{\partial^{2}\mathcal{E}(\mathbf{u},\lambda)}{\partial\mathbf{u}\partial\mathbf{u}}\right]_{\begin{pmatrix}\mathbf{u}\\(\lambda_{c}),\lambda_{c}\end{pmatrix}} \text{ non - invertible at } \overset{0}{\mathbf{u}}(\lambda_{c}) \implies \text{ principal solution singularity}$$
$$[\mathcal{E}^{c}_{,\mathbf{u}\mathbf{u}}] \begin{bmatrix} \mathbf{u}\\ \mathbf{u}\end{bmatrix} = \mathbf{0}, \ i = 1, ..., m; \quad \lambda_{c}: \text{ critical load, } \overset{(i)}{\mathbf{u}}: \text{ critical mode, } m: \text{ multiplicity}$$
$$\text{if : } [\mathcal{E}^{c}_{,\mathbf{u}\lambda}] \begin{bmatrix} \mathbf{u}\\ \mathbf{u}\end{bmatrix} = \mathbf{0} \implies \text{ bifurcation at } \lambda_{c}$$
$$\text{if : } [\mathcal{E}^{c}_{,\mathbf{u}\lambda}] \begin{bmatrix} \mathbf{u}\\ \mathbf{u}\end{bmatrix} \neq \mathbf{0} \implies \text{ limit load at } \lambda_{c}$$
$$\overset{1}{\mathbf{u}} = \overset{1}{\mathbf{u}} \implies \overset{1}{\mathbf{u}} = \overset{1}{\mathbf{u}} \implies \overset{1}{\mathbf{u}} = \overset{1}{\mathbf{u}} \xrightarrow{\overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} = \overset{1}{\mathbf{u}} \implies \overset{1}{\mathbf{u}} \xrightarrow{\overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} = \overset{1}{\mathbf{u}} \implies \overset{1}{\mathbf{u}} \xrightarrow{\overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}} \overset{1}{\mathbf{u}}} \overset{1}{\mathbf{u}} \overset$$

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### LSK (LYAPUNOV - SCHMIDT - KOITER) ASYMPTOTICS

• General asymptotic method to study motion of systems (discrete or continuous) near singular points. Here the method is applied to the equilibrium of conservative elastic systems.

• IDEA: Study the projection of equilibrium equations along the finite dimensional null space of the system's stability operator at critical point. This way the study of a large problem is reduced to the study of a nonlinear system of *m* equations, where *m* is the multiplicity of the stability operator's eigenvalue at the critical point.

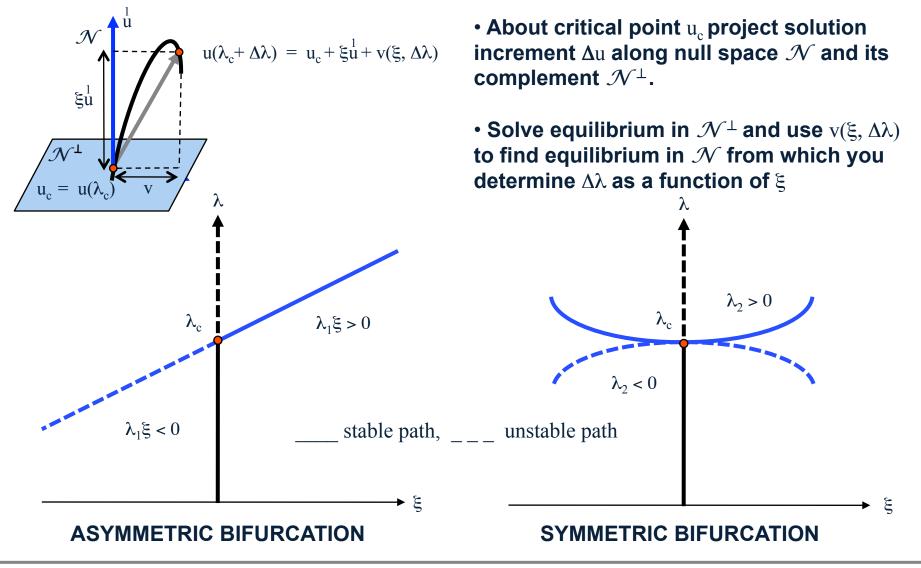
• Method follows asymptotically equilibrium paths emerging from bifurcation points (simple or multiple) of perfect systems and determines their stability.

• Method also investigates the equilibrium and stability of imperfect systems, near critical points of their perfect counterparts, for small imperfection amplitudes.

• NOTE: Method is useful in determining post-bifurcation behavior and imperfection sensitivity in applications as well as in providing efficient numerical tools for finding solutions near the singular points of complex nonlinear systems.

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#### **ASYMPTOTIC EXPANSIONS – SIMPLE BIFURCATION CASE**

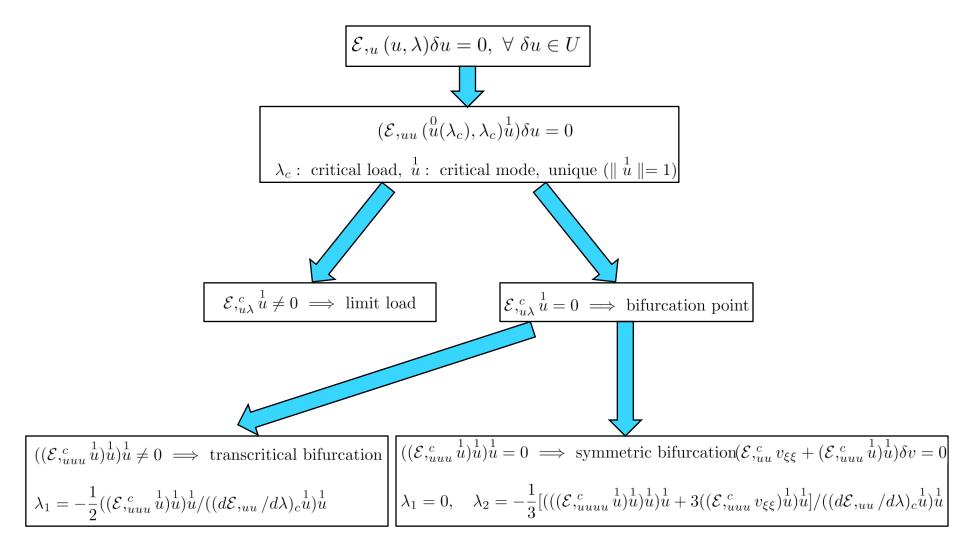


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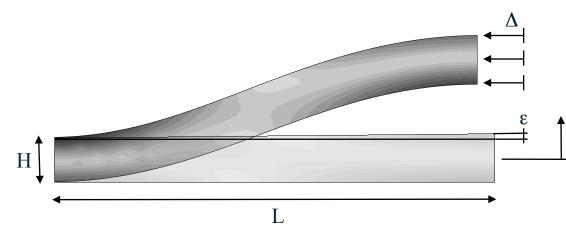


### **ASYMPTOTIC EXPANSIONS – SIMPLE BIFURCATION CASE**





### **CONCEPT OF IMPERFECTION – ILLUSTRATION**



0.016 0.014 0.012 0.010 ∆ / L 0.008 0.006 0.004 0.002 0 000 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 w / H  $\rightarrow$   $\varepsilon$  = 0.05  $\rightarrow$   $\varepsilon$  = 0.1  $\rightarrow$   $\varepsilon$  = 0.2  $\bullet$  critical strain

Beam slenderness: L/H = 10

Imperfection  $\varepsilon = \Delta H/H$ 

NOTE: Different types of imperfections can be used, geometric or material – all are equivalent

Deformation of an axially compressed beam that has a slight geometric imperfection (beam is trapezoidal with an imperfection angle  $\epsilon = \Delta H/H$ )

W

As imperfection amplitude  $\epsilon$  decreases, equilibrium approaches perfect case





### LSK ASYMPTOTICS – IMPERFECTIONS – SIMPLE MODE

• Behavior of imperfect structure near critical load can be analyzed by asymptotic expansion of equilibrium solution.

• **Bifurcation** point in perfect case is **replaced** by **limit points** in imperfect case.

• Method determines the limit points (where stability changes) of imperfect structure and the load drop  $\Delta \lambda_s$  from the critical load of the perfect structure  $\lambda_c$  to the maximum load of the imperfect one  $\lambda_s$ .

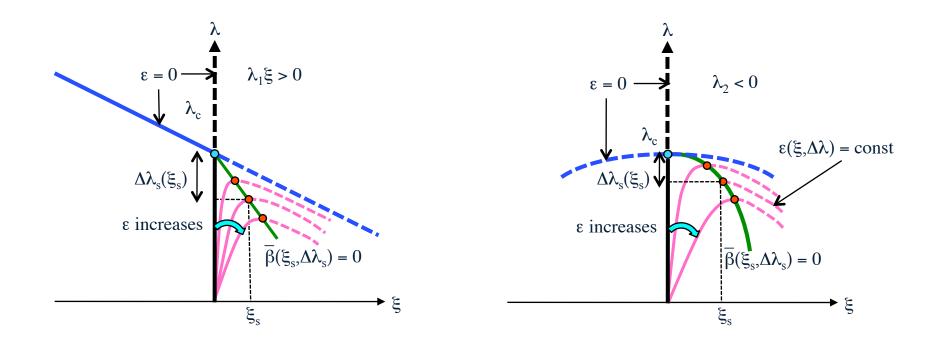
- Recall that in real structures the amplitude  $\epsilon$  can be controlled but not the shape w.
- Load drop is maximized when imperfection has the shape of the eigenmode.

• Structures are imperfection sensitive (i.e.  $\Delta \lambda_s < 0$ ) for asymmetric or symmetric subcritical bifurcations (load max exists for the equilibrium path through zero load);  $\Delta \lambda_s = O(\epsilon^{1/2})$  for asymmetric case and  $\Delta \lambda_s = O(\epsilon^{2/3})$  for subcritical symmetric case.

• NOTE: Imperfection can occur in any property (material or geometric) that destroys the symmetry of the system; all related asymptotic analyses are equivalent.



#### **IMPERFECTIONS – SIMPLE MODE – GENERAL RESULTS**



Asymmetric bifurcation – Imperfect Case

Symmetric bifurcation – Imperfect Case



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### **ASYMPTOTIC EXPANSIONS – MUTIPLE BIFURCATION CASE**

• Interest of multiple mode case for applications: systems with an initially high symmetry: e.g. cylinder buckling, stability of cubic crystals.

• IDEA: Study the projection of equilibrium equations along the finite dimensional null space of the system's stability operator at critical point. This way the study of a large problem is reduced to the study of a nonlinear system of *m* equations where *m* is the multiplicity of the stability operator's eigenvalue at the critical point.

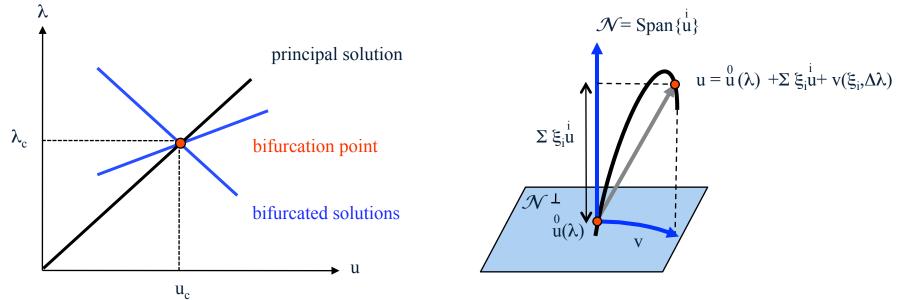
• Method follows asymptotically all the equilibrium paths emerging from the bifurcation point of the perfect system and determines their stability.

• Method also investigates the equilibrium and stability of imperfect systems, near critical points of their perfect counterparts, for small imperfection amplitudes

•NOTE: Method is useful in determining post-bifurcation behavior and imperfection sensitivity in applications as well as in providing efficient numerical tools for finding solutions near the singular points of complex nonlinear systems with a high degree of initial symmetry



### **ASYMPTOTIC EXPANSIONS – MUTIPLE BIFURCATION CASE**



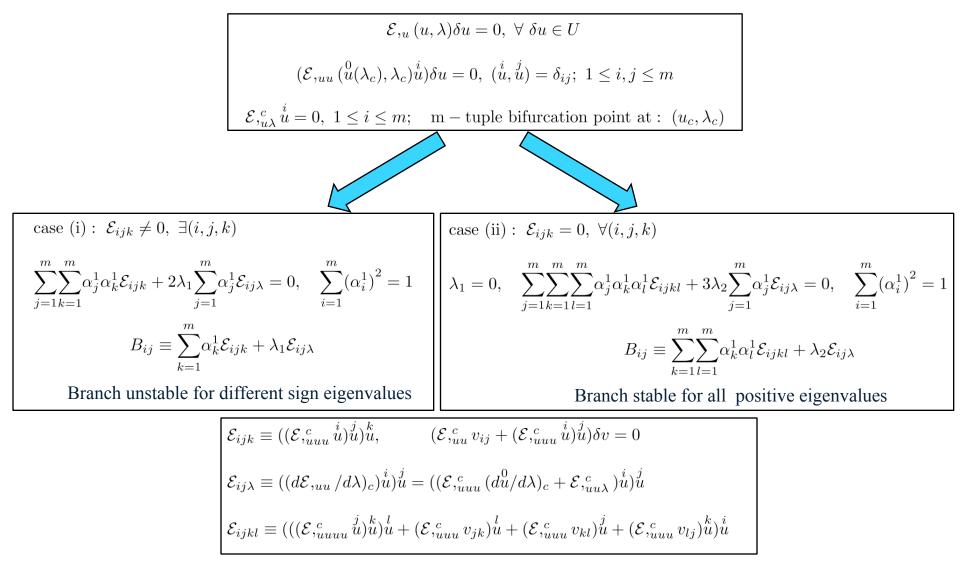
Method is a straightforward generalization of simple mode case:

• About an arbitrary point  $\lambda = \lambda_c + \Delta \lambda$  of the principal solution  $u^0(\lambda)$  project difference  $\Delta u = u - u^0$  along *m*-dimensional null space  $\mathcal{N}$  and its orthogonal complement  $\mathcal{N}^{\perp}$ . Subsequently expand corresponding equilibrium equations about  $\lambda_c$ 

• From critical point  $u_c$ ,  $\lambda_c$  at most  $2^m$ -1 (asymmetric case) or  $(3^m$ -1)/2 (symmetric case) bifurcated equilibrium paths emerge (because initial tangents are solutions of  $m \ 2^{nd}$  or  $3^{rd}$  order polynomial equations with m variables



#### **ASYMPTOTIC EXPANSIONS – MUTIPLE BIFURCATION CASE**





## STABILITY OF CONTINUA AND NUMERICAL (FEM) METHODS

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### NUMERICAL (FEM) TECHNIQUES IN STABILITY PROBLEMS

• Using the Finite Element Method (FEM), problem's principal solution at load  $\lambda$  is obtained using an incremental Newton-Raphson algorithm. Method, which starts from zero load – zero displacement, always converges for adequately small load step  $\Delta\lambda$  and gives equilibrium solution to any accuracy required.

• At any given load  $\lambda$ , method automatically calculates corresponding stability operator, which is the tangent stiffness matrix  $K(\lambda)$ .

• Solution technique uses K = LDU (Cholesky) decomposition. Presence of critical points (i.e. limit load/bifurcation point) on the principal solution imply zeros in the diagonal matrix D (i.e.  $(D_{ii})_{min}(\lambda_c) = 0$ ).

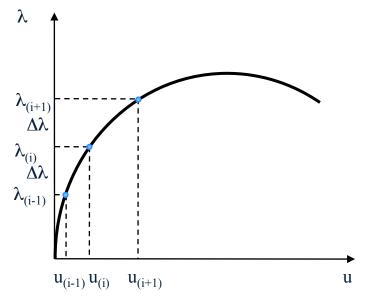
• **Bisection** method is used to accurately find the critical load.

• If the critical load is an *m*-tuple bifurcation point, the *m* lowest entries of D are zero at the critical load.

• If the critical load is a limit point, arc-length continuation methods are used to go past this point.

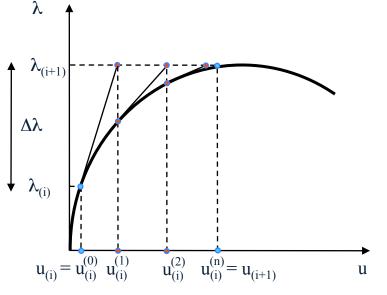


### **INCREMENTAL NEWTON-RAPHSON METHOD**



Equilibrium solutions (principal/ bifurcated) of continuum problems amenable to finite d.o.f. case through discretization techniques (FEM)

Incremental method starting from zero load/displacement is needed to guarantee convergence of N-R (for small enough load steps)



N-R method finds equilibrium solutions and stability operator K.

K=LDU decomposition of stability operator – available as part of the solution procedure – in combination with bisection gives critical points

LSK asymptotics used to start bifurcated paths



#### FEM DISCRETIZATION OF NONLINEAR EQUILIBRIUM

 $\mathcal{E}(u,\lambda)$ : continuum energy at displacement  $u(\mathbf{x}) \in U$  and load  $\lambda \geq 0$ 

 $\mathcal{E}(\mathbf{u}, \lambda)$ : discretized energy at displacement  $\mathbf{u} \in \mathbb{R}^n$  and load  $\lambda \ge 0$ 

 $\mathbf{u} = \{u_i\}_{i=1}^n$ :  $u(\mathbf{x}) = \sum_{i=1}^n u_i \varphi_i(\mathbf{x}), u_i$ : d.o.f,  $\varphi_i(\mathbf{x}) \in U$ : basis function

F.E.M. method :  $\varphi_i(\mathbf{x})$  have compact support, by using element shape functions

ADVANTAGE :  $\mathcal{E}_{,uu}$  is banded matrix, i.e. populated about its diagonal

 $\mathcal{E}_{,\mathbf{u}}(\mathbf{u},\lambda) = \mathbf{0}: \quad \partial \mathcal{E}/\partial u_i = 0, \ i = 1 \dots n:$  equilibrium equations

Start at :  $\lambda = 0$ ,  $\mathbf{u} = \mathbf{0}$ 

Continue by : Incremental Newton – Raphson Method



#### **INCREMENTAL NEWTON-RAPHSON METHOD**

 $\mathrm{Newton-Raphson\ method}:\ \mathbf{0}=\mathcal{E}_{,\mathbf{u}}\left(\mathbf{u}+\Delta\mathbf{u},\lambda\right)\approx\mathcal{E}_{,\mathbf{u}}\left(\mathbf{u},\lambda\right)+\mathcal{E}_{,\mathbf{uu}}\left(\mathbf{u},\lambda\right)\Delta\mathbf{u}\implies$ 

$$\mathbf{u}_{(i)}^{(1)} - \mathbf{u}_{(i)}^{(0)} = -[\mathcal{E}_{,\mathbf{u}\mathbf{u}} (\mathbf{u}_{(i)}^{(0)}, \lambda_{(i)})]^{-1} \mathcal{E}_{,\mathbf{u}} (\mathbf{u}_{(i)}^{(0)}, \lambda_{(i+1)}),$$

start at  $\mathbf{u}_{(i)}^{(0)} = \mathbf{u}_{(i)} \equiv \mathbf{u}(\lambda_{(i)})$ , where  $\mathbf{u}_{(i)}^{(j)}$ : **u** at increment (i) and iteration (j)

$$\mathbf{u}_{(i)}^{(j+1)} - \mathbf{u}_{(i)}^{(j)} = -[\mathcal{E},_{\mathbf{u}\mathbf{u}} (\mathbf{u}_{(i)}^{(j)}, \lambda_{(i+1)})]^{-1} \mathcal{E},_{\mathbf{u}} (\mathbf{u}_{(i)}^{(j)}, \lambda_{(i+1)}),$$

end at  $\mathbf{u}_{(i)}^{(j+1)} = \mathbf{u}_{(i+1)} \equiv \mathbf{u}(\lambda_{(i+1)})$ , if error is small :  $\|\mathcal{E}_{\mathbf{u}}(\mathbf{u}_{(i)}^{(j)}, \lambda_{(i+1)})\| < \varepsilon$ 

STABILITY CHECK : positive definiteness of  $\mathcal{E}_{,uu} = LDU$  (Choleski decomposition)

 $\mathbf{L}$ : lower triangular,  $\mathbf{L}^T = \mathbf{U}$ : upper triangular,  $\mathbf{D}$ : diagonal, matrices

 $\mathcal{E}_{,\mathbf{u}\mathbf{u}}(\mathbf{u}(\lambda),\lambda)$  positive definite at load  $\lambda \iff D_{ii}(\lambda) > 0, \ \forall \ 1 \le i \le n$ 



## **RELATION BETWEEN STABILITY & MICROSTRUCTURE**

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### **STABILITY APPLICATIONS AT DIFFERENT SCALES**

- Structural (bars, plates)
- Materials (composites, honeycomb microstructural scale)
- Solids (phase transformation atomistic scale)

**NEW CONCEPT: Local** (order of unit cell dimensions) vs global (order of overall structural dimensions) modes

**NEW TOOL** (for stability of infinite, perfectly periodic structures)

**Bloch waves** (continuum)

Phonon spectra (discrete)

**Bounded** solutions of differential equations with periodic coefficients are of the type:  $u(x) = \exp(i\omega x) p(x)$  where p(x+L) = p(x) (*L* period of coefficients)

**BIG ADVANTAGE:** Only the smallest unit cell needs to be considered in calculations



### **COMPRESSION-INDUCED FAILURE IN CELLULAR SOLIDS**

• To model the entire deformation history of a cellular solid under compression, one has to solve for a finite-size structure (boundary effects are important) with many unit cells, using an elastoplastic constitutive law (unloading is important). In addition, initial imperfections have to be used, with different imperfection shapes often giving very different results.

• However, the onset of the first instability during the load increase in an infinite, perfect structure can be found accurately from the principal solution, by using one unit cell.

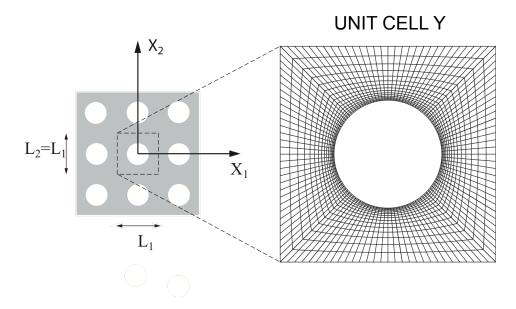
• The use of only a unit cell in finding the first instability occurring in a loading process is guaranteed from Bloch wave representation theorem for the solution of a system of linear differential equations with periodic coefficients. The Bloch wave representation theorem is the generalization to PDE's of Floquet's theorem for ODE's with periodic coefficients.

• The Bloch wave representation theorem is easily adapted to cellular geometry.

• The use of an elastic model in calculations for elastoplastic solids is based on the assumption that in the principal solution, all cell walls satisfy loading condition as load increases, thus using a deformation theory of plasticity (which has a stored energy).



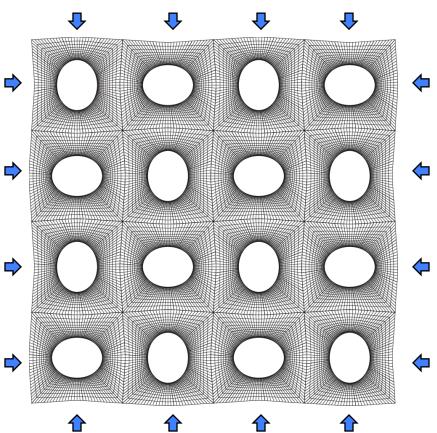
## STABILITY OF INFINITE PERIODIC SOLIDS: BLOCH WAVE



• The Y-periodic, principal solution of infinite, perfect solid is initially stable.

• Upon load increase, the system bifurcates with modes that are no longer Y-periodic.

• Critical load and corresponding eigenmode can be found based on calculations on one unit cell Y with the help of Bloch wave representation theorem.



First bifurcation mode of a porous, compressible neo-Hookean solid ( $W = 0.5[\mu(I_2-2-lnI_2)+(\kappa-\mu)(\sqrt{I_2-1})^2]$ ) loaded under compressive, equi-biaxial plane strain ( $E_{II} = E_{22} = -\lambda$ ). The critical load is  $\lambda_c = 8\%$ 



### STABILITY OF INFINITE PERIODIC SOLIDS: BLOCH WAVE

$$\overset{0}{\beta}(\lambda) = \min_{\delta u \in U} \left[ (\mathcal{E}_{,uu} (\overset{0}{u}(\lambda), \lambda) \delta u) \delta u \right], \ ||\delta u|| = 1; \text{ stability of } \overset{0}{u}(\lambda)$$

 $\overset{0}{u}(\lambda) = Y - \text{periodic (unit cell } Y) : \overset{0}{u}_{i,j}(X_k + n_k L_k) = \overset{0}{u}_{i,j}(X_k) (!); n_k \in \mathbb{N}.$ 

$$(\mathcal{E}_{,uu}^{0} \delta u) \delta u = \int_{V} \left\{ \left[ \frac{\partial^{2} W}{\partial F_{ij} \partial F_{kl}} \right]_{u}^{0} \delta u_{i,j} \delta u_{k,l} \right\} dV; \quad \delta u_{i,j} \equiv \partial \delta u_{i} / \partial X_{j}, \ V = \mathbb{R}^{2} \text{ or } \mathbb{R}^{3}$$

$$\forall \ \delta u \in U: \quad \delta u_j(\mathbf{X}) = \delta p_j(\mathbf{X}) \exp(i\omega_k X_k): \text{ BLOCH WAVE THEOREM.}$$
  
where:  $\omega_k L_k \ (!) \in (0, 2\pi); \quad k = 1, 2 \text{ if } V = \mathbb{R}^2 \text{ or } k = 1, 2, 3 \text{ if } V = \mathbb{R}^3$ 

$$\delta \mathbf{p} = Y - \text{periodic}: \quad \delta p_j(X_k + n_k L_k) = \delta p_j(X_k) \ (!); \quad n_k \in \mathbb{N}.$$

$${}^{0}_{\beta}(\lambda) = \inf_{\boldsymbol{\omega}} \left[ \min_{\delta \mathbf{p}} \int_{Y} \left\{ \left[ \frac{\partial^{2} W}{\partial F_{ij} \partial F_{kl}} \right]_{u}^{0} \overline{\delta u}_{i,j} \delta u_{k,l} \right\} dV \right]; \text{ calculations need only } Y$$

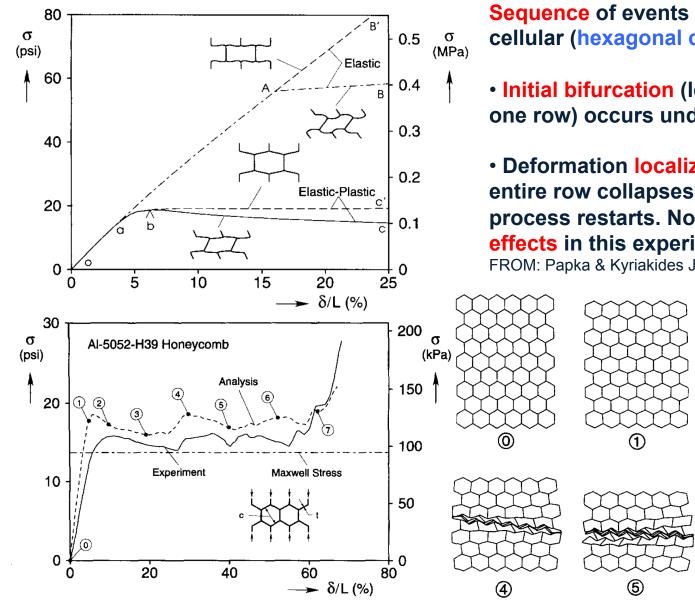


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Sequence of events in 2D loading of a cellular (hexagonal cells) solid:

- Initial bifurcation (local mode, involving one row) occurs under reduced loads.
- Deformation localizes in that row until entire row collapses (contact) and the process restarts. Notice strong boundary effects in this experiment.

FROM: Papka & Kyriakides JMPS, 1994, 42, pp. 1499-1532

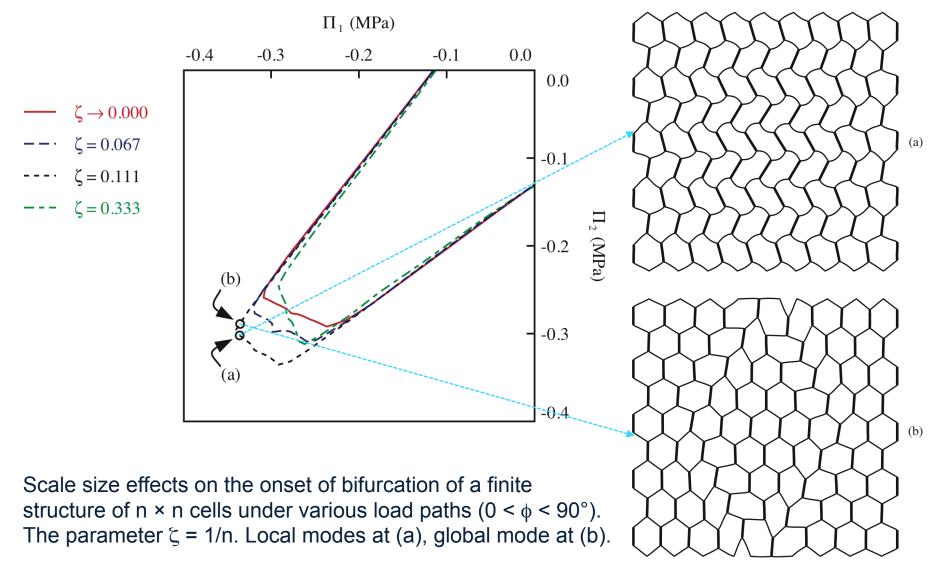
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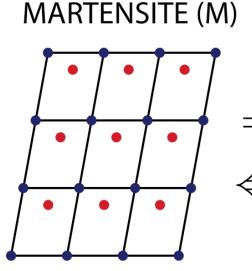


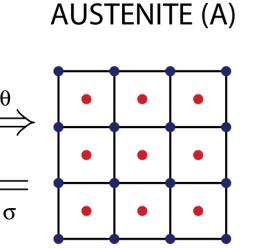
### HEXAGONAL HONEYCOMB: LOCAL AND GLOBAL MODES





#### PHASE TRANSFORMATIONS: LATTICE INSTABILITIES





θ

 Shape memory behavior due to instabilities of the atomic lattice:

 At higher temperatures: austenitic (higher symmetry phase) is stable.

 At higher stresses: martensitic (lower) symmetry phase) is stable.

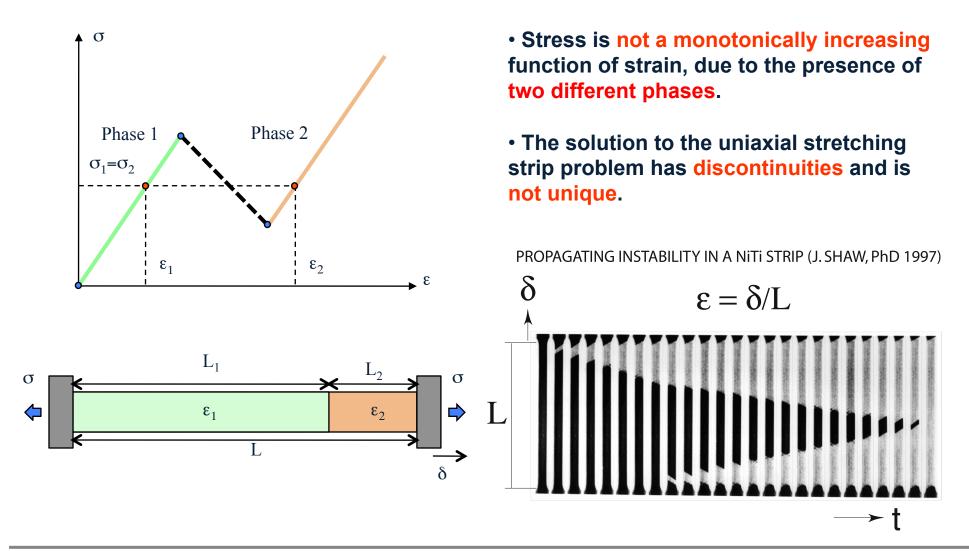
(lower symmetry)

(higher symmetry)

 The consequence of this lattice-level instability shows all the way up to structural scale.

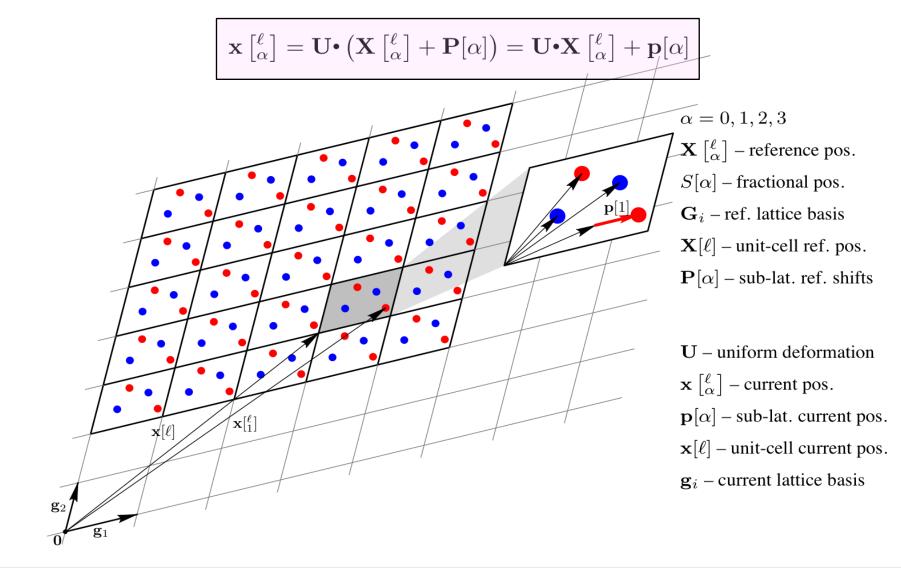


#### PHASE TRANSFORMATIONS: MACROSCOPIC MODELING





### PHASE TRANSFORMATIONS: ATOMISTIC MODELING





### **CAUCHY-BORN HYPOTHESIS: EQUILIBRIUM & STABILITY**

- Equilibrium:  $\frac{\partial \widetilde{W}}{\partial \mathbf{u}} = \mathbf{0} \left\{ \begin{array}{c} \frac{\partial \widetilde{W}}{\partial \mathbf{U}} = \mathbf{0}, \\ \frac{\partial \widetilde{W}}{\partial \mathbf{S}[1]} = \mathbf{0}, & \frac{\partial \widetilde{W}}{\partial \mathbf{S}[2]} = \mathbf{0}, \\ \frac{\partial \widetilde{W}}{\partial \mathbf{S}[2]} = \mathbf{0}, & \frac{\partial \widetilde{W}}{\partial \mathbf{S}[3]} = \mathbf{0}. \end{array} \right.$
- Stability for perturbations of ∞ wavelength):
  - Cauchy-Born stability (local energy minimizer):

$$\delta \mathbf{u} \frac{\partial^2 \widetilde{W}}{\partial \mathbf{u} \partial \mathbf{u}} \delta \mathbf{u} > 0; \qquad \delta \mathbf{u} = \{ \delta \mathbf{U}, \delta \mathbf{S}[1], \delta \mathbf{S}[2], \delta \mathbf{S}[3] \}, \ \delta \mathbf{U} = \delta \mathbf{U}^T.$$



## PHONON STABILITY FOR INFINITE, PERFECT LATTICE

• Linearized equations of motion about equilibrium:

$$m_{\alpha} \ddot{\mathbf{u}} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} = -\sum_{\begin{bmatrix} \ell' \\ \alpha' \end{bmatrix}} \mathbf{K} \begin{bmatrix} \ell & \ell' \\ \alpha & \alpha' \end{bmatrix} \cdot \mathbf{u} \begin{bmatrix} \ell' \\ \alpha' \end{bmatrix},$$

 $m_{\alpha}$  – mass of atom  $\alpha$ ,

$$\mathbf{u} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} - \text{displacement of atom } \alpha \text{ in unit cell } \ell,$$
$$\mathbf{K} \begin{bmatrix} \ell & \ell' \\ \alpha & \alpha' \end{bmatrix} - \text{stiffness between atoms } \begin{bmatrix} \ell \\ \alpha \end{bmatrix} \text{ and } \begin{bmatrix} \ell' \\ \alpha' \end{bmatrix} \text{ cal-culated from the atomic potentials.}$$

• Initial conditions:

$$\mathbf{u} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} \Big|_{t=0} = \mathbf{u}^0 \begin{bmatrix} \ell \\ \alpha \end{bmatrix}, \quad \dot{\mathbf{u}} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} \Big|_{t=0} = \dot{\mathbf{u}}^0 \begin{bmatrix} \ell \\ \alpha \end{bmatrix}.$$

• Stability (in the sense of Lyapunov):

$$\left\|\mathbf{u}^{0}\left[{}^{\ell}_{\alpha}\right]\right\|, \left\|\dot{\mathbf{u}}^{0}\left[{}^{\ell}_{\alpha}\right]\right\| < \epsilon \implies \left\|\mathbf{u}\left[{}^{\ell}_{\alpha}\right]\right\|, \left\|\dot{\mathbf{u}}\left[{}^{\ell}_{\alpha}\right]\right\| < \delta(\epsilon).$$



### PHONON STABILITY FOR INFINITE, PERFECT LATTICE

• Phonon (normal mode) solutions: (*a*-lattice spacing, M = 4-atoms/unit-cell)

$$\mathbf{u} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} = \mathbf{\Delta} \mathbf{u}^{(q)}[\alpha] \exp \left\{ -i \left( \mathbf{k} \cdot \mathbf{X} \begin{bmatrix} \ell \\ \alpha \end{bmatrix} + \omega^{(q)}(\mathbf{k}) t \right) \right\},\$$

$$\mathbf{k} - \text{wave number vector, } \mathbf{k} \in \left[ -\frac{\pi}{a}, \frac{\pi}{a} \right]^{3};\$$

$$q - \text{phonon index, } q = 1, 2, \dots, 3M;\$$

$$\omega^{(q)}(\mathbf{k}) - \text{phonon frequency};\$$

$$\mathbf{\Delta} \mathbf{u}^{(q)}[\alpha] - \text{amplitude vector.}$$

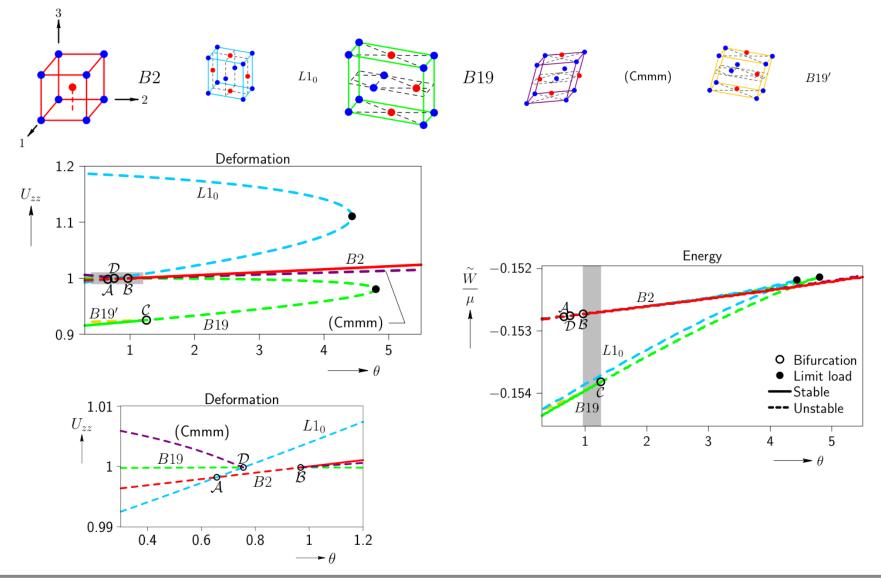
• Phonon-stability:

$$\left(\omega^{(q)}(\mathbf{k})\right)^2 > 0$$
, for all  $\mathbf{k}$ , and all  $q$ .

PHONON STABILITY FOR DICRETE SYSTEMS IS SAME TO BLOCH WAVE FOR CONTINUA



### PHONON STABILITY FOR INFINITE, PERFECT LATTICE



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### SOME FINAL COMMENTS

- Thank you for taking class and following up especially for my morning lecture devotees
- Hope key concepts & new ideas from this class remain with you long after details forgotten
- Encourage you to stop by with questions, comments and suggestions on how to improve class
- My office door wide open for those of you interested in this area and willing to learn more – I am welcoming you to do research in this area (and a thesis if interested...)