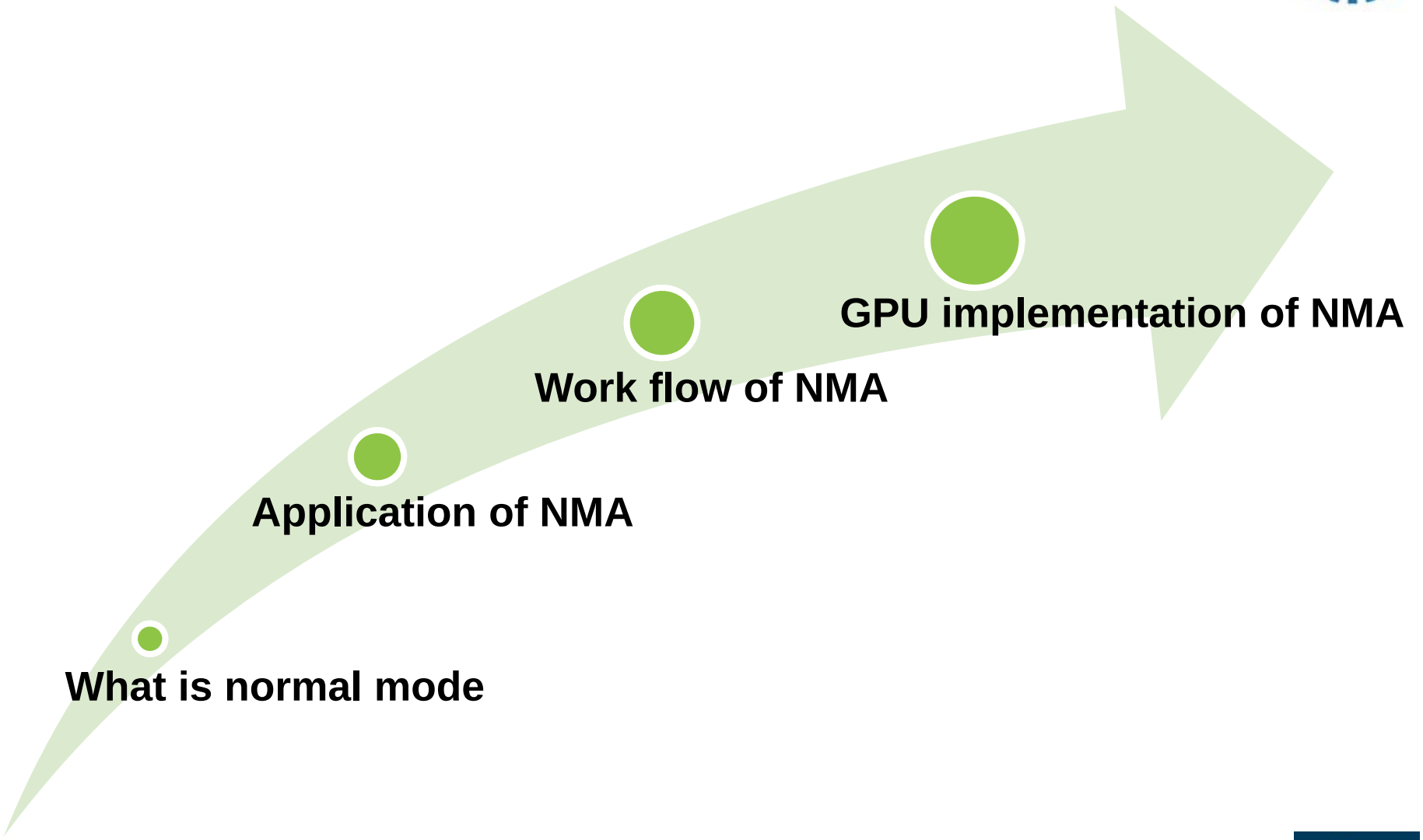
All-atom normal mode analysis (NMA)

Dongsheng Lei
Molecular Foundry, Lawrence Berkeley National Laboratory
Department of Applied physics, Xi'an Jiaotong University
TCBG GPU Workshop, 08/04/2013

Outline



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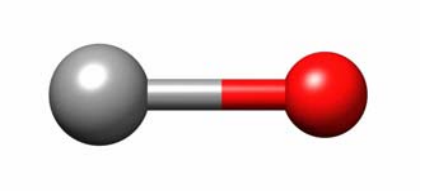
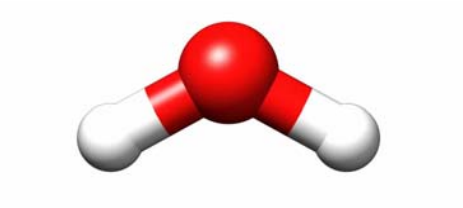
Normal mode

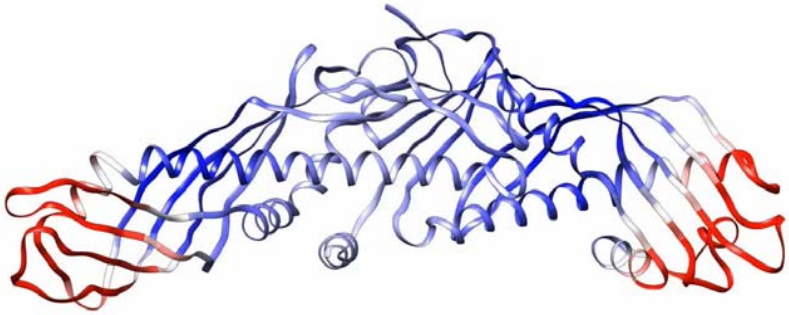
Normal mode: a motion pattern in which all atoms of molecule move with the same frequency and a fixed phase.



Bond stretching



Angle bend



Collective motion of protein

***Mode*:** harmonic motions
***Normal*:** modes are independent of each other

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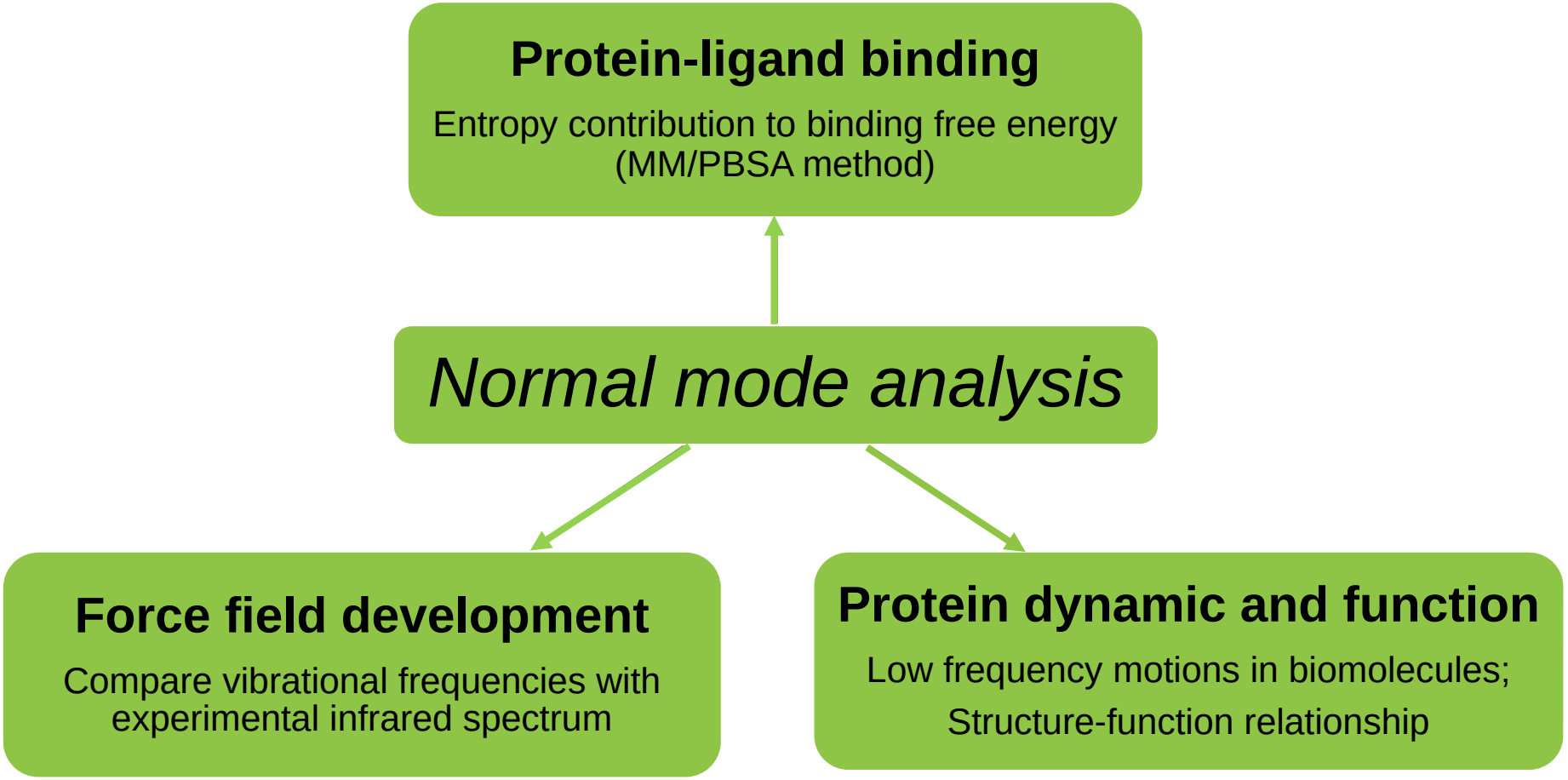
Application of normal mode analysis



All-atom normal mode analysis

Energy minimization

"Hessian" matrix

$$H = \begin{bmatrix} \frac{\partial^2 U}{\partial x_1^2} & \cdots & \frac{\partial^2 U}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 U}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 U}{\partial x_n^2} \end{bmatrix}$$

Second order derivatives of potential

Mass weighted hessian matrix

Diagonalization of the matrix

Eigenvalues: Vibrational frequencies

Eigenvectors: Movement directions

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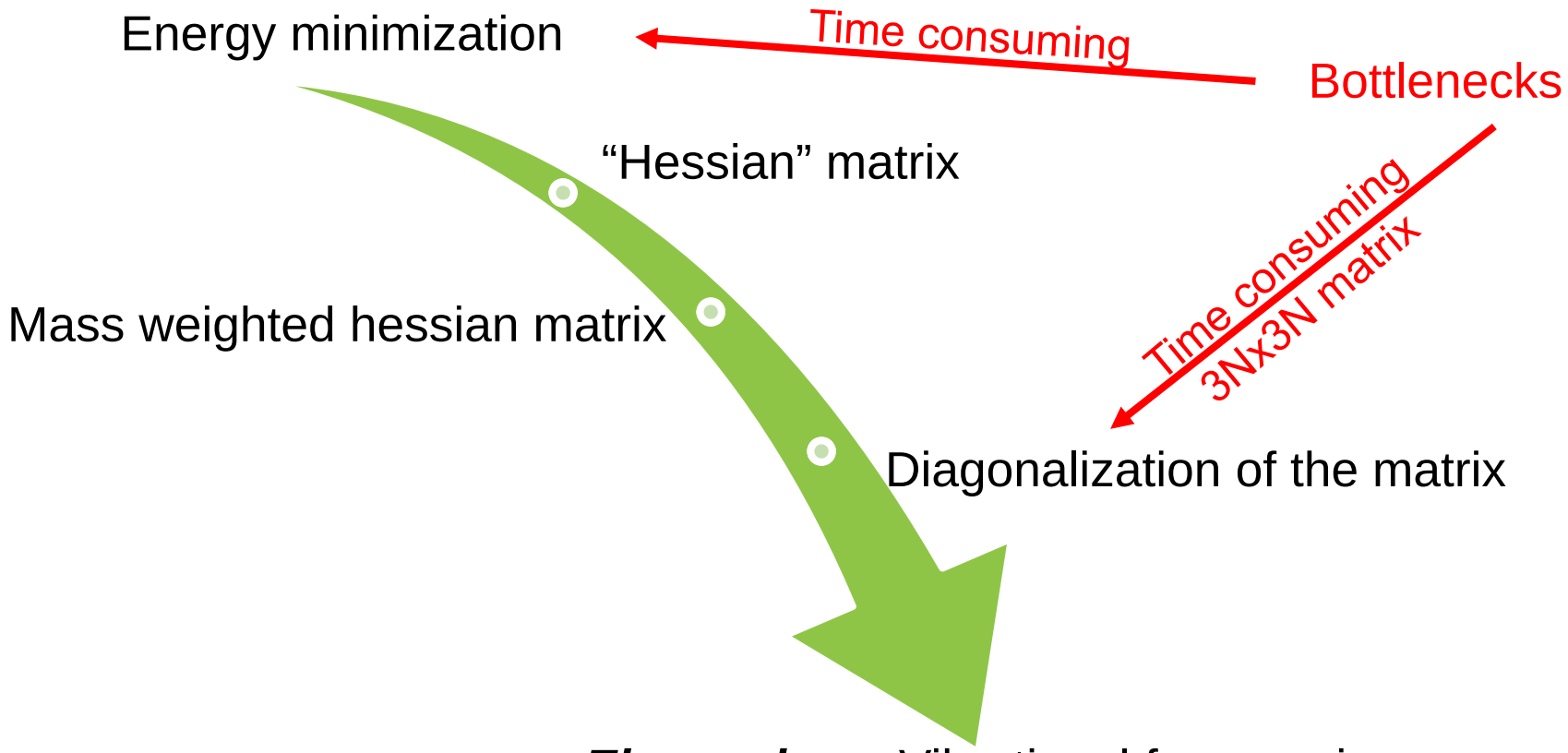
All-atom normal mode analysis



Eigenvalues: Vibrational frequencies

Eigenvectors: Movement directions

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GPU implementation of NMA

Energy minimization: GPU-accelerated NAMD

Calculation of “Hessian” matrix: GPU parallelization

Diagonalization: Householder-QR transformation on GPU

1 A standalone module for performing NMA with NAMD and CHARMM force field.

2 Extending this application to other user defined force field.

- Challenges: Diagonalization of hessian matrix demands much computer memory. Thousand atoms will require few Gigabytes of memory.

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Thank you!

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