李俊

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2023 年应届生

教育经历

上海交通大学 2016年9月-2022年12月

- 物理学　博士　GPA　3.54/4
- 荣誉奖项：物理天文学院2017年学术大会优秀海报奖、物理天文学院优秀助教(2018)

四川大学 2012年9月-2016年06月

- 物理学　本科　排名3/45
- 工商管理　本科(双学位)　排名8/119

项目经历

1. 蛋白质的老化动力学

- 项目简介： 蛋白质动力学对其引起的疾病机理理解至关重要。利用Linux开源软件对蛋白多粒子系统进行分子动力学模拟，统计分析均方位移、自关联行为等特征，首次发现蛋白质动力学具有非平衡态的老化Aging行为。
- 发表论文： Jun Li, Thomas Neusius, Micholas Dean Smith, Aljaž Godec, Liang Hong, Ralf Metzler and Jeremy C. Smith*. "Reply to: Insufficient evidence for ageing in protein dynamics." ***Nature Physics*** (影响因子20.0), 17.7 (2021): 775, 第一作者, 已接收

2. 单分子SHP2蛋白的非遍历动力学

- 项目简介： 运用全内反射光学显微镜和计算机模拟，研究SHP2蛋白在10^{-12} ~10^{2}秒时间尺度的运动，证明每个蛋白分子的运动行为各不相同，即具有非遍历性。这有助于理解为什么每个蛋白酶活性、催化效率、运动等性质有所不同。
- 论文成果：Jun Li, JingFei Xie, Aljaž Godec, Keith R. Weninger, Jeremy C. Smith, Liang Hong*. "Non-ergodic internal dynamics of a globular protein observed over fourteen orders in time." ***Nature Communications*** (影响因子14.9), 第一作者, 准备审稿

3. 生物大分子的次扩散运动

- 项目简介： 利用计算机模拟研究六种生物大分子(DNA/蛋白)运动，发现起次扩散机制依赖于分子的大小，对于尺寸较小的分子(如:小于2纳米DNA)由分数阶布朗运动主导，而大蛋白分子的是属于连续时间随机游走模型。
- 论文成果：Jun Li, Liang Hong*. "The role of ergodicity, aging to resolve the origin of molecules diffusion." 第一作者, 准备审稿

4. 镁离子诱导RNA折叠是熵驱动的

- 项目简介： 单分子显微镜观察到RNA在有镁离子情形下，其结构展示出更大的灵活性并折叠部分结构。进行等温量热滴定实验从热力学的角度证明，Mg^{2+}对RNA的折叠是熵驱动的，这也解释了为什么RNA在有镁离子时具有更大的灵活性。
- 论文成果：Jun Li, Liang Hong* & Yu Liu*. "Entropic driven of Mg^{2+} induced RNA riboswitch folding." 第一作者, 准备投稿

5. 分子的构象社交网络特征研究与对比

- 项目简介： 用k-mean算法对白/DNA/高分子等六类分子结构聚类定义出微观态，然后可将运动轨迹可视化成一个态转移社交网络。对网络特征进行分析发现，结构球蛋白的社交络是分形高阶的，而无结构的高分子构象网络是平坦且简单的。
- 论文成果：Jun Li, Liang Hong*. "Energy landscape of biomolecules revealed by transition network." 第一作者, 准备投稿

6. 其他论文(非第一作者)

- Tan, Pan, **Jun Li**, and Liang Hong*. "Properties for diffusion of hydration water on protein surface." Physica B: Condensed Matter (2019).
- Liu, Zhuo, **Jun Li**, et al. "Direct experimental characterization of contributions from self-motion of hydrogen and from interatomic motion of heavy atoms to protein anharmonicity." *The Journal of Physical Chemistry B* 122.43 (2018): 9956-9961.

7. 课题组网站设计

- 项目简介：从零设计和建设研究生课题组网页(https://ins.sjtu.edu.cn/people/lhong)，后续进行了更新、日常维护等工作。

其他信息

- 技能证书：Matlab(★★★★)、Linux(★★★)、Python(★★★)、英语(CET-6)、Photoshop(★★★)、Zemax(★★)
- 社会实践：视觉中国签约摄影师(2019-)，物理学习委员(2014-2016)，工商管理班长(2013-2016)，课程助教(2016-2021)

个人总结

- 直博五年级在读，有一定的编程基础和数据挖掘能力
- 专业成绩优秀，具备较强的学习能力和适应能力

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EDUCATION

Shanghai Jiao Tong University *Seqt.2016 - June.2021*

- PhD in Physics | GPA 3.54/4
- Awards: 2017 Academic Conference Excellent Poster Award

Sichuan University *Seqt.2012 - June.2016*

- B.S. in Physics | GPA 3.4/4
- B.S. in Business Administration | GPA 3.6/4
- Awards: Single first-class scholarship (2016)、Outstanding student leaders (2016)

PROJECT

Reply to: Insufficient evidence for ageing in protein dynamics

- Abstract: Internal motions of proteins are essential to their function. The time dependence of protein structural fluctuations is highly complex, manifesting subdiffusive, non-exponential behaviour with effective relaxation times existing over many decades in time, from ps up to $\sim 10^2$ s. Here, using molecular dynamics simulations, we show that, on timescales from 10^{-12} to 10^{-5} s, motions in single proteins are self- similar, non-equilibrium and exhibit ageing. The characteristic relaxation time for a distance fluctuation, such as inter-domain motion, is observation-time-dependent, increasing in a simple, power-law fashion, arising from the fractal nature of the topology and geometry of the energy landscape explored. Diffusion over the energy landscape follows a non-ergodic con- tinuous time random walk. Comparison with single-molecule experiments suggests that the non-equilibrium self-similar dynamical behaviour persists up to timescales approaching the in vivo lifespan of individual protein molecules.
- Publication: **Jun Li**, Xiaohu Hu, Thomas Neusius, Micholas Dean Smith, Aljaž Godec, Liang Hong, Ralf Metzler, and Jeremy C. Smith. "Reply to: Insufficient evidence for ageing in protein dynamics." ***Nature Physics***, 17.7 (2021): 775

Non-ergodic internal dynamics of a globular protein observed over fourteen orders in time

- Abstract: By performing single-molecule experiments and MD simulations on a multi-domain protein in its folded globular state, we demonstrate protein internal dynamics can be non-ergodic over fourteen orders in time, longer than the characteristic catalytic time of the protein. This finding significantly recasts existing ideas in molecular biophysics that connect ensemble-averaged protein dynamics to biological function. Instead, non-ergodicity splits the population of otherwise identical proteins into subpopulations with drastically distinct conformations, flexibilities, and reaction rates over timescales longer than associated with their biological function.
- Manuscript: **Jun Li**, JingFei Xie, Aljaž Godec, Keith R. Weninger, Cong Liu, Jeremy C. Smith, Liang Hong. "Non-ergodic internal dynamics of a globular protein observed over fourteen orders in time." ***PNAS*** (impact factor 11.2), under review.

The role of ergodicity, aging, and Gaussianity to resolve the origins of biomolecules subdiffusion

- Abstract: The internal motions of biomolecules are essential to facilitate their function. Although biological macromolecules had been conventionally shown subdiffusion dynamics, only recently has the subdiffusion been associated with non-ergodicity. New questions have been stimulated by these findings in biophysics and statistical mechanics. Is non-ergodic subdiffusion a general strategy shared by biomolecules? Which underlying mechanisms hold responsible for it? Here, we perform extensive molecular dynamics (MD) simulations to characterize the internal dynamics of six biomolecules and resolve mixed origins of their motions. We observe Gaussian shape propagator, and ergodic subdiffusion in the small biological system (i.e., single-stranded DNA, double-stranded DNA, and a single- domain protein KRAS), strong consistency with fractional Brownian motion (FBM). While in multi-domain protein (PGK, SHP2) and an intrinsically disordered protein (SNAP-25), we show that these proteins undergo anti-correlated, non-ergodic, and aging dynamics at the timescale of nanoseconds. The further statistical analysis underscores the mixing of continuous-time random walk (CTRW) and FBM playing a major role in their internal dynamics.
- Manuscript: **Jun Li**, Pan Tan, Song Li, Liang Hong. "The role of ergodicity, aging, and Gaussianity to resolve the origins of biomolecules subdiffusion." First author, to be submitted.

Energy landscape of various macromolecules revealed by transition network analysis

- Abstract: The energy landscape of macromolecules holds responsible for their specific functions and underlying dynamics. To overcome the main drawbacks of reaction-coordinate-based methods, we visualize the underlying potential energy surface (PES) of various molecules from all-atom molecular dynamics (MD) simulations, represented by a complex network of conformations transitions between the corresponding metastable states. The topological and geometrical property of energy landscape for six molecules, e.g., globular protein (SHP2 and PGK), intrinsically disordered protein (IDP), double-stranded DNA (dsDNA), single-stranded DNA (ssDNA), and polymer (poly N-diethylacrylamide, PDEA), are investigated by explicit water MD simulations and transition network analysis. The complex network features characterized by the methods of box covering algorithm, loop length, and average path length, indicate that the dsDNA and a globular protein's energy landscape are high- dimensional and fractal. Whereas the non-compact molecules (ssDNA, IDP, polymer) are one-dimensional and straightforward. This difference between folded proteins, dsDNA, and coil-like molecules suggests the folded molecules have a "funnel-shaped" global energy minimum. In contrast, the disordered molecules have multiple local energy minima separated by small barriers flat.
- Manuscript: **Jun Li**, Liang Hong. "Energy landscape of biomolecules revealed by transition network." First author, to be submitted.

Other publications (not first author)

- Tan, Pan, **Jun Li**, and Liang Hong. "Properties for diffusion of hydration water on protein surface." Physica B: Condensed Matter (2019).
- Liu, Zhuo, **Jun Li**, et al. "Direct experimental characterization of contributions from self-motion of hydrogen and from interatomic motion of heavy atoms to protein anharmonicity." *The Journal of Physical Chemistry B* 122.43 (2018): 9956-9961.

Other

- Skills**:** Matlab(familiar)，Python(basic), Linux(basic)、Photoshop(basic)、Zemax(limited)