formalism, might be related to negative cooperative phenomena. Based on our studies with Ompr^* mutants, we propose that the underlying mechanism is a competitive binding of cations and protons occurring in the narrow central constriction of the channel. Temperature-controlled experiments suggest that the entropic benefit arising from cooperative interactions is the driving force behind the pH sensitivity of the channel.

1367-Pos Board B137
New Parallelized DelPhi: Fast and Efficient Poisson-Boltzmann Solver to Calculate Electrostatics of Large Supramolecular Structures
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Electrostatic potential in systems comprised of biological macromolecules and water phase is described by a 2nd order elliptic partial differential equation, known as the Poisson-Boltzmann equation (PBE). DelPhi is a PBE solver (http://compbio.clemson.edu/delphi.php) which adopts finite difference method to solve this equation numerically and has been widely recognized in the biological community due to its efficiency and accuracy. In this work, we introduce an efficient parallel computing technique via the unique implementation of Gauss-Seidel iteration method in DelPhi. The implementation allows for dynamics partitioning of the multiprocessing jobs by decision making algorithm which takes into account the available computing resources associated with a particular computer cluster. Further we demonstrate the advantages of the new parallelized DelPhi by computing the electrostatic potential and the corresponding energies of large supramolecular structures and molecular motors. The work is supported by NIH, NIGMS, grant number 1R01GM093937-01.

1368-Pos Board B138
Single Molecule Studies of Streptavidin-Biotin Dissociation at Elevated Temperatures
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Over the past few years single molecule spectroscopic techniques have matured and are widely used in the biomolecular sciences. More recently, temperature control has been incorporated, increasing the dimensionality of the possible experimental parameters. However, conventional immobilization techniques rely on biotin-streptavidin linkages to localize single molecules on surfaces. While this ligand binding interaction is one of the strongest non-covalent linkages in nature (KD = 10^-14 M) and is extremely stable at room temperature, the kinetics of dissociation at elevated temperatures are poorly understood. Pulsed laser based IR absorbance heating and fluorescence techniques are used to measure the dissociation rate at temperatures well above room temperature. The rate constants of dissociation are found to increase significantly from ~2x10^-5 s^-1 at 20°C to ~1x10^-3 s^-1 at 55°C. Eyring analysis reveals that the dissociation reaction has a large enthalpic contribution (\Delta H = 20 (1) kcal/mol), the magnitude of which is on the order of the previously measured enthalpies of formation. This result indicates that the biotin binding occurs over a nearly barrier-less transition state.

1370-Pos Board B140
Rate Constants are Variables in Almost all Chemical Reactions
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Chemical reactions are almost always analyzed using rate constants assumed to be constants. Rate constants are constant if reactants do not interact and have zero excess free energy of interaction, and if spatial gradients are insignificant. Reactants in biology almost always interact strongly because charges attract or repel. Biology occurs in mixtures of ions and organic acids and bases with large permanent charge. Large partial charges are found in carbonyl, amine, and peptide bonds of biomolecules and in the solvent water itself. The energy of one charged reactant depends on all charge in the ionic atmosphere around that reactant. The atmosphere contains all species and so the energy of reactants depends strongly on the concentrations of all species with significant charge. Measuring excess free energy of interactions has been the life’s work of generations of physical chemists. Rate constants in life’s solutions should not be assumed constant when physical measurements show important excess interaction energy. ‘Everything’ interacts with everything in those cases and rate constants are variables. When rate constants are assumed to be constant, interactions of reactants can be mistaken for conformational changes or complex reaction schemes of an enzyme. Physical models provide alternatives that reflect known properties of ions in confined spaces. Physical models of L-type Ca channels, DEKA Na channels, and most notably Ryanodine Receptors, account for experiments, over five orders of concentration, in mixtures of many species. Anomalous Mole Fraction Effects were predicted by Gillespie in Ryanodine Receptors before they were found experimentally by Meissner and Xu. The variational calculus provides an alternative description of interactions. The Energy Variational Approach of Chen Liu [Journal Chemical Physics (2010) 133:104104] is mathematically well-defined, even unique (for a given physical model). It includes interactions and spatial gradients that allow flow.

1371-Pos Board B141
Observed Fibonacci Sequences in the Periodic Table
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C. H. Waddington: “…how genotypes become translated into phenotypes? … Selection does not impinge directly on genotypes, but on phenotypes” [Annals of NYAS v.231, 1974, pp.32-42]. At the 54th Annual Meeting [Biophysical J. v.98. Issue 3, p.659a] we showed that the Fibonacci Sequence specifically maps the 20 Aminos and their corresponding 64 Codons distributed in the 4x4 Genetic Tableau (1969), and also 6x6 DO Group of Proteins (Waddington-Thom Epigenetic Landscape). Nucleic Acids (C, G, U, A) are elements of phenotypes (C, N, O, H), and finally Elements are phenotypes of Orbitals as genotypes. In this presentation, we show that, in the Periodic Table, specific orbitals of certain elements signal topological characteristics of the formation of biomolecules. The group of elements, their (Fibonacci) numbers, and topological characteristics are: 1 - 0 : {Space Origin}; 5 - 1 : {p: Dynamics by Bonding}; 24, 29 - 2 : {d: (Convergence mod 6) and Hexagon}; 42, 44, 45, 46 - 3 : {t: (Asymmetric Triangle)}; 57, 58, 64, 78, 79 - 5 : {f to d and t: (Non-orientable Mobius Band)}; 89, 90, 91, 92, 93, 96, 110, 111, 118 - 7 {d to f and a: (Non-orientable Klein Bottle)}. The Periodic Table indicates a helical growth that creates a hyperbolic surface.

1372-Pos Board B142
Enzymatic Characterization and Spectroscopic Studies of Diarylthene Modified Lysozyme
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Photochromic compounds such as azobenzenes, and diarylenethenes change their chemical and physical properties reversibly with their structural change by photo irradiation. This photoresponsive character may be useful for regulation of physiological functions of biomaterials, analysis of their reaction mechanism, and development of function materials. Previously, we have reported that photoresponsive lysozymes modified with azobenzenes at a position-specific residue (Lys 33, or Lys 116) in hen egg white lysozyme, and their enzymatic properties were reversibly modulated according to photosomarization of azobenzene moiety. In this study, diarylenethene derivatives having substituted phenyl group at 5-position of the thiophene ring were used as a photochromic moiety. Hen egg white lysozyme was modified at Lys 33, which is located in the vicinity of the substrate-binding site. The influence of photochromism of diarylenethene moiety on enzyme kinetics and the fluorescence, and transient absorption spectroscopy were studied to clarify the photo regulation mechanism. In MALDI TOF mass analysis of modified diarylenethenes and their reduced triptic peptides, it is revealed that a diarylenethene binds to Lys33 on lysozyme through amide binding. The modified lysozymes exhibited photochromic behavior, and the enzyme kinetics parameters were modulated reversibly according to photochromism. Enzyme reactions were assayed using cell wall of Micrococcus lysodeikticus as a substrate. In the case of modified lysozyme using 1, 2-(5-carboxypheny-2-methylthiophene-3-yI)-cyclopentene as a diarylenethene moiety, the catalytic efficiency undergo drastically change reversibly; the value in photo-stationary state at 313 nm reduced by about one-twentieth of that of the open form. The binding constant with a substrate analogue (tri-N-acetyl-D-glucosamine) was also reduced by isomerization from open form to closed form. The efficiency of energy transfer to xanthene derivatives, and NMR