PRIMEX 1.0 and VPCR 2.0: Processing genomic sequence data for efficient and accurate simulation of PCR reactions with genomic DNA as template - (session: Novel Algorithms for Bioinformatics)

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Increased availability of genomic sequence data provides space for bioinformatic tools utilizing these large datasets in novel applications. We have set out to automate the prediction of PCR reaction products using arbitrary primers and genomic DNA as template. While this may seem a trivial task for a well-designed pair of primers, the task becomes much more challenging in a wide range of special situations. Firstly, the search for primer annealing sites becomes prohibitively slow on large genomes with currently available tools. Secondly, a mathematical model of the PCR reaction is required to simulate amplification in cases where primers go through a wide range of states besides the desired binding to the target sequence (unspecific binding, secondary structure formation), or where several amplification products compete for polymerase activity (multiplex PCR). We present a set of programs that address these problems and rapidly predict the outcome of any PCR reaction. PRIMEX is a tool that can find all relevant primer-binding sites in a single genome in a fraction of a second. VPCR is a set of routines that analyze the output provided by PRIMEX and run a dynamic mathematical model of the PCR amplification process. We will show our first results that compare VPCR output and real PCRs performed in the laboratory.