PRIGO: Parallel Robotics Inspired Goniometer for Protein Crystallography

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Abstract

This paper presents a novel goniometer which is designed for use with X-ray diffraction analysis in protein crystallography. The PRIGO (Parallel Robotics Inspired Goniometer) is a 6 degree of freedom positioning device, allowing 3 translations (x, y, z) and 3 rotations (Omega, Chi, Phi) of a sample around a Tool Centre Point (T.C.P.), placed in the crystal to be scanned. The structure is a hybrid of serial and parallel kinematics. This approach allows new possibilities for sample orientation in protein crystallography.

1 Introduction

The collection of X-ray diffraction data in protein crystallography relies upon a complex experimental setup. The classical rotation method consists in rotating a crystal placed in an X-ray beam about an axis (called OMEGA) passing through the crystal itself. The beam diameter can be as small as 5um. Typical crystal dimensions range from a few microns to some hundreds of micrometers. The Bragg diffraction of the beam is collected with a large planar pixel detector, placed behind the sample. Higher data quality can be obtained by performing these scans with the crystal placed in different orientations with respect to the Omega axis. The delicate reorientation of the crystal, keeping its X, Y, Z coordinates unchanged is generally performed using an Eulerian Cradle [Fig.1] or a Kappa-Goniometer [1]. However, existing Eulerian Cradle and Kappa-Goniometers do not fulfill the many constraints imposed by the experimental setup. Available space is limited, and the workspace has an inconvenient shape. During data acquisition, the mechanical structure must not interrupt the X-Ray beam, otherwise self-shadowing will occur, resulting in invalid measurement results. Traditional goniometers suffer from limited angular ranges, inconvenient dimensions, limited accuracy and self shadowing issues.

2 The PRIGO Concept

The project was an effort to rethink and reevaluate traditional Goniometer concepts for this specific application. The result is a fully motorized 6 degree of freedom positioning device, allowing 3 translations (SHx,SHy,SHz) and 3 rotations (OMEGA, CHI, PHI) of the sample around a given point (TCP). It is based upon a combination of serial and parallel kinematics, and emulates the traditional Eulerian cradle goniometer design (also refered to as 'the arc').

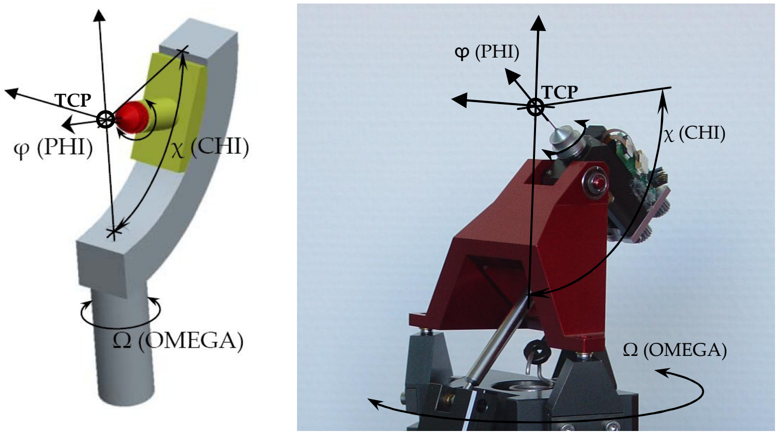

Figure 1: The Eulerian Cradle or ‘Arc’, and how it is emulated with PRIGO. In addition, PRIGO can adapt to different sample holder sizes, maintaining the sample in the TCP.

3 Kinematics

The kinematics chain consists of 1 rotation OMEGA, followed by 4 linear sliders working synchronously to synthesize the three translations SHx,SHy,SHz and a rotation CHI. Finally the PHI rotation rotates the sample around the sample holder axis.

Each of the three legs consist of a motorised linear translation (resolution ~1µm), a flexure rotary joint and a spherical joint, which connects to the tetrahaedron. This sequence is equal for all three legs, but with the pivot axes rotated by 120° [Fig.2].

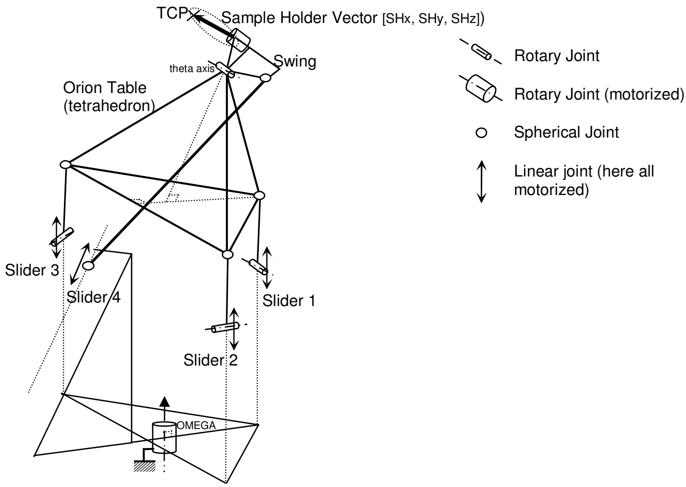

Figure 2: Kinematic structure of PRIGO

This basic kinematic structure resembles that of the Orion [2], and is used to position the swing's theta axis (the parasitic tilt angles are acceptable for this application). A fourth slider tilts the swing via a rod with two spherical joint ends. This way the swing can be positioned and orientated in space. The swing also accomodates the motorised phi rotation. The whole structure is held together with a global tension spring, which also acts as an eliminator for play in the entire structure.

With linear strokes of 60/60/60/100 mm for the sliders and 360° for Phi & Omega rotations, the following workspace can be covered:

Translations:	SHx, SHy, SHz:	[-5mm, +5mm] with 2um resolution
Rotations:	OMEGA:	[-inf, +inf] with 1 arc-sec resolution
	CHI:	[0, 90°] with 1 mrad resolution
	PHI:	[-inf, +inf] with 1mrad resolution

4 Control System

PRIGO's control system is written on the Orchestra Control Engine [3], an open source real-time control framework running on RTAI/Linux. This transparent and flexible system allowed a powerful implementation of the control system with a low cost multipurpose card and off the shelf PC components. The whole control system including motor amplifiers were fitted into a 3U 19” rack unit. All 5 axis can be moved synchronously and the control loop runs at 1kHz.

5 Geometrical Model (FK-IK Calculations)

A central goal was to allow crystallographers to operate the device using their traditional coordinate systems. To allow a fast and intuitive use of the device, it was decided to do all trajectory generation in user coordinates, so that movements really resemble the emulated Eulerian cradles. This required that forward and inverse kinematic models be calculated in real time, and be included within the control loop. Due to the complexity of the task, the inital Matlab model took well over 1 ms to calculate. Many optimisations were made and the model was finally coded in C++, without using dynamic memory allocation. Calculation times could be reduced down to avg. 75µs for the IK and 30µs for the FK model, on an Intel Celeron M550 CPU.

6 Results

A first prototype was constructed and tested at the Swiss Light Source. A first sphere of confusion could be measured of around 30 µm. This was larger than expected, not all dimensions used in the geometrical model could be measured to a micron precise. Notably the flexure joints were simple blades, and yet were represented in the model as pure rotations. A next step was taken to calibrate the movements. Under a controlled environment, the sphere of confusion could be reduced to below 10µm.

7 Conclusions

PRIGO has proven to be a very interesting alternative for all applications where Eulerian Cradles and Kappa-Goniometers are used today. A second version, building upon the promising results and experiences of the prototype, is currently being designed.

8 Acknowledgements

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