

First Results from PRIGO III, the Parallel Robotics Inspired Goniometer for Protein Crystallography

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Abstract

In this paper we present the implementation and measurement results of the six degree of freedom manipulator design PRIGO III. It represents a novel goniometer approach for the use at protein crystallography beamlines at synchrotrons. The concept was presented at the 2009 EUSPEN conference [1], and meanwhile a working prototype of PRIGO III is in use at the Swiss Light Source.

We give a short overview of the design work: optimisation of the geometrical model, FEM calculations compared to the measurement results, and applied techniques for metrology will be explained.

1 Short introduction to the PRIGO concept

PRIGO is in essence a 6 degree of freedom positioning device, based on parallel kinematics, which emulates an Eulerian cradle multi-axis goniometer (also known as 'the arc'). It can be seen as an alternative to classical Kappa and Eulerian Cradle goniometers, when limited space is an issue. The three rotation angles OMEGA, CHI & PHI are of main importance for crystallographers, and will be referred to further on. For details on the kinematic structure, see [1].

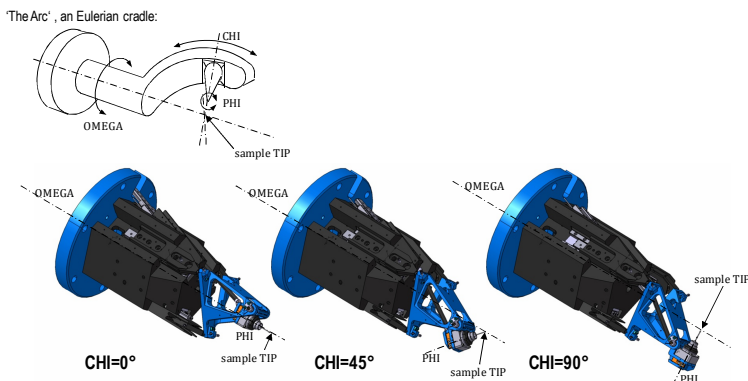


Figure 1: PRIGO emulates 'the arc'

2 PRIGO III

Motivation for the development of a new prototype of PRIGO started after the evaluation and testing of piezo stick & slip linear stages produced by SmarAct GmbH. The compact form factor, with built-in linear encoders allowed us to optimize the geometry to a level previously never achieved.

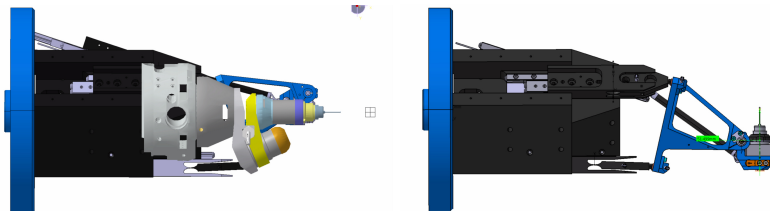


Figure 2: PRIGO III side view, Left: superimposed with MiniKappa (ESRF) [2], at CHI=0°, Right: at CHI=90°

Due to the compact phi rotation stage, the detector can get as close as 60mm for all orientations, without collision.

3 Geometry Optimisation

For the development this prototype, we had a well studied kinematics model, which could be extensively used to perform kinematics analyses. Geometrical parameters could be tuned, and from a given workspace, the required actuator ranges could be deduced. At the same time resolution transmission ratios could be observed. Singularities could be identified and avoided. Maximum ball joint and flexure angles could be pre-calculated. Initialization routines could be simulated.

With parallel kinematic structures, the motor's resolution is often not distributed homogeneously throughout the workspace. There can be regions where the motor resolution translates to a high resolution at the sample level, and there are regions where the resolution is worse, especially around singularities.

In the last prototype of PRIGO, a shortcoming was identified: when at CHI=0°, the sample position (TIP) resolution was not very good. This was made even worse, because mostly the device is used at CHI=0°, and only in certain occasions, larger CHI angles are used. Therefore a re-optimisation of the geometry was done, to improve the resolution for CHI=0°.

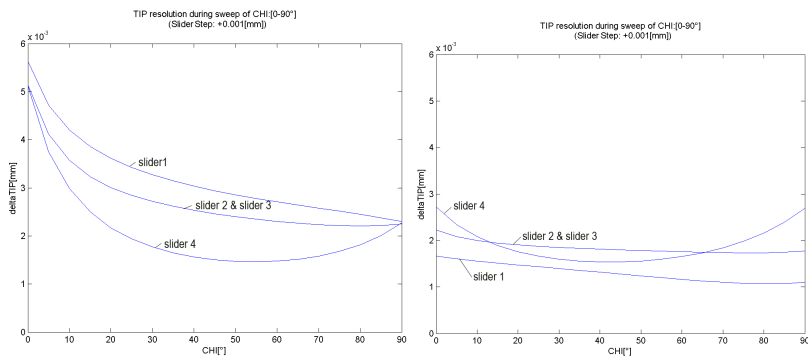


Figure 3: Tip resolution during sweep of CHI:[0-90°] Left: PRIGO II (last prototype) Right: PRIGO III (new prototype)

4 FEM analysis of deflection at the sample position

The application requires that PRIGO be mounted horizontally. An FEM analysis was done to estimate the deflection at the sample position, for different postures. 4 postures were chosen: CHI=0° with gravity acting in Y, CHI=0° with gravity acting in X directions. And then the same again for CHI=90°. The largest flexure was observed at CHI=90° in Y, the calculated deflection being 3.1 µm.

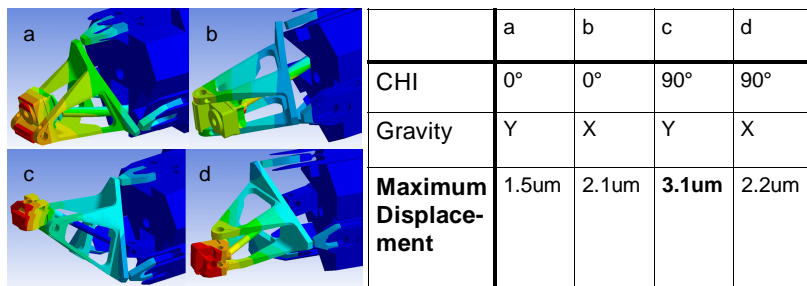


Figure 4: FEM analysis of deflection with horizontal mounting

This value was mainly used as an indication of the order of magnitude of the deflection; it is in fact the relative deflection throughout a revolution of OMEGA which is important for the application. Nevertheless this provided a good qualitative method to compare solutions amongst each other.

5 Measurements of deflection at the sample position

Once the device was assembled, a measurement of the sample TIP deflection was done. The sample was replaced by a 0.5” steel ball (roundness <0.25µm), which position was measured by two capacitive sensors in horizontal and vertical direction.

The ball was rotated around the OMEGA axis, and centred until the sinusoidal component with periodicity of 360° was eliminated.

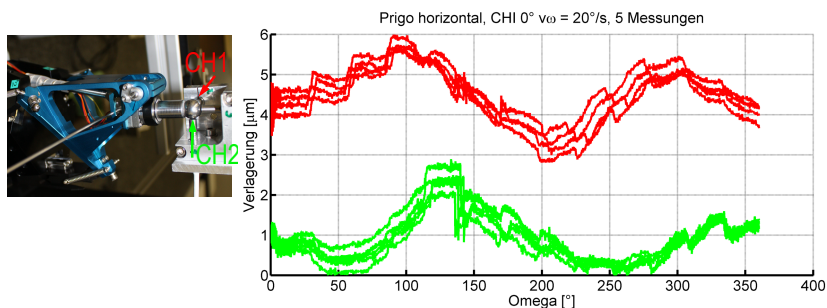


Figure 5: TIP deflection

The measured deflection at the sample position was found to deviate less than 3µm for a rotation around OMEGA. Crystallographers often refer to this value as the Sphere of Confusion (SOC) for the OMEGA rotation. A SOC of below 5µm was required, so the specifications were well achieved.

6 Shortcomings of the geometrical model and calibration of the CHI axis

A remaining problem is the sphere of confusion around the CHI axis. This is because it is a virtual axis which depends on the accuracy of the geometrical model in the control system. So far we have not been able to measure all functional lengths of the model, and are looking into calibration strategies for the CHI rotation.

7 Conclusions

A working prototype of PRIGO with a Sphere of Confusion of OMEGA of <3µm has been developed, is in use at beamline X06DA at Swiss Light Source.

8 Acknowledgements: We would also like to thank Urs Ellenberger, Urs Bugmann and the workshop for the machining of the parts, and Xinyu Wang for her FEM calculations.

References:

- [1] W. Gletting et al.: “PRIGO: Parallel Robotics Inspired Goniometer for Protein Crystallography”, Proceedings of the 9th euspen International Conference, San Sebastian, Spain, June 2nd - 5th, 2009, Volume1, p.192
- [2]. F.Cipriani, S. Brockhauser, R. Ravelli.: MK2 – miniKappa goniometer head, Jan2006, <http://www.embl-grenoble.fr/groups/instr/MK2.pdf>