



UNITED DEVICES™

THE UNIVERSITY OF OXFORD: Intel and United Devices Team Up to Speed Cancer Research Grid MP Case Study

The Customer

The University of Oxford Chemistry Department is home to the Centre for Computational Drug Design, set up by the National Foundation for Cancer Research (NFCR).

The Challenge

Oxford's aggressive goal was to screen several chemical libraries against 12 target proteins previously determined to be key elements in cancer growth. The objective was to dramatically increase the scope of large-scale virtual screening, speeding the search for drug candidates while maintaining a highly manageable and secure research environment.

Phase I: Initial Execution and Results

"No other single technology partner has accelerated our recent research as dramatically as United Devices."

Dr. Sujuan Ba, Science Director,
National Foundation For Cancer
Research

In the initial phase of the project, Oxford worked with United Devices to enable a third-party virtual screening application on the Grid MP platform. Participants from all over the globe donated the spare

computational cycles of their PCs and servers to the project – over 1 million machines contributed processing power to Grid MP Global to perform the screening.

By the end of the first month, Grid MP-driven technology had exceeded expectations by screening an unparalleled 15,000 molecules every second. Researchers quickly took advantage of the flexibility and

Summary

Increasingly, life science breakthroughs depend on the ability to sift through immense amounts of data to find meaningful information. Discovery and market success now rely more on access to substantial computational power than any other factor.

The Intel-United Devices Cancer Research Project demonstrates how the Grid MP platform can improve the scope and speed of drug discovery. The project highlights the security, scalability and manageability of Grid MP as it dramatically accelerates the research process using a commercially available screening application on the United Devices Global Grid.

scalability of Grid MP Global to expand the project's scope, in order to capitalize on these unexpectedly rapid results. An estimated 3.5 billion molecules were eventually screened against the 12 target proteins, making this the largest computational chemistry project ever undertaken.

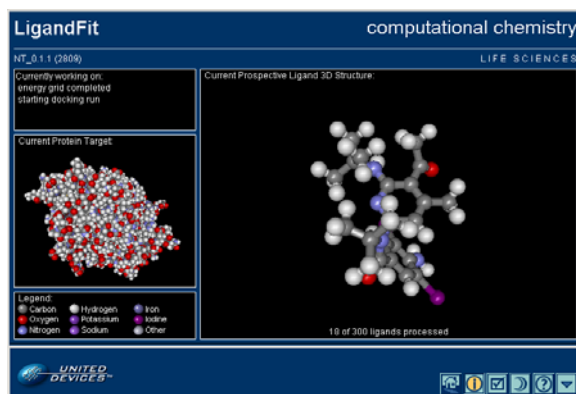
In six months, the project had uncovered 800,000 ranked hits, completing a combined total of nearly 80,000 computational years of work. This work was fueled exclusively by the combination of the United Devices' Grid MP solution and the global aggregation of under-utilized computational power.

“Massively distributed computing has allowed databases of billions of compounds to be screened against protein targets in a matter of days.”

Dr. Graham Richards
University of Oxford

Phase II: Continuing Success

After the overwhelming success of the project's first phase, Oxford and NCFR researchers began a second phase to continue this groundbreaking research. The second phase uses Accelrys' high-throughput docking and scoring application, LigandFit, running on Grid MP Global to refine the research results from Phase I.



In Phase II, LigandFit will screen the massive number of “hits” produced in Phase I to more accurately predict and prioritize the suitability of these hits as potential lead candidates for drug development.

“Our obvious next step is to take the hits generated so far and produce a smaller list of more accurate hits, thus leading to a more tractable set of potential drugs to synthesize and test in the labs,” says Dr. Graham Richards, Chair of the Oxford Chemistry Department.

The project's second phase, which has attracted over 1.9 million volunteers, has already completed nearly 43 years of compute time for the LigandFit screening. When complete, the screening will produce a list of promising drug candidates for synthesis and testing, which will require further experimental collaborators from both academia and industry.

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