

# A grand vision for configurable science and minimizing the loss model

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## The respondents



**Mark J. Emkjer (MJE, pictured)** is president and CEO of Accelrys, Inc. He has more than twenty-five years of management experience, most recently as president and chief operating officer of Sunquest Information Systems, Inc., a clinical data management solutions provider. During his tenure at Sunquest, he more than doubled earnings per share and

cash, resulting in a doubling of the stock price, and successfully completed the sale of Sunquest to Misys PLC for over \$400 million. Prior to joining Sunquest, he was president and chief executive officer of Pace Health Management Systems, Inc., where he increased revenue by 50% and successfully sold Pace to 3M Corporation. He holds a BS in Finance and an MBA from Florida Atlantic University and the University of Miami, respectively.



**Frank K. Brown (FKB, pictured)** has spent the last 20 years of his career innovating new scientific methods in the field of computational science and informatics and applying them in commercial pharmaceutical enterprises. From 1997 to 2006, he held positions of increasing responsibility at Johnson & Johnson, and, most recently, was a senior research fellow within the office of the CIO. He received his Ph.D. in physical organic chemistry from the University of Pittsburgh under the direction of Ken Houk and did postdoctoral studies in biophysics at UCSF under the direction of Peter Kollman. He has published over 50 peer-reviewed papers and is the named holder of two patents. He is a past chairman of ACS COMP Division and is also recognized as the person who first defined the term “chemoinformatics”.

## Questions and answers

- WAW:** Has SciTegic “disappeared”? The Web site has gone and all the SciTegic solutions have been incorporated into the Accelrys site.
- FKB:** The company has gone but the name remains as a brand, for example in SciTegic Enterprise Server, our scientific business intelligence platform. Matt Hahn is still here.
- MJE:** Matt Hahn has a new position. As VP of R&D he is responsible for making IT solutions work, in an agile development environment. Frank is chief

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science officer. He solves customers' problems; he creates new solutions. Incidentally, there are three times as many programmers now in "Sci-Tegic" than there used to be.

WAW: I like your new Web site but some of the old hands may think that you have hidden the names of their favorite products: Cerius2, Insight, QUANTA, Ludi, Catalyst, CHARMm, etc.

FKB: You can find all those products if you search for them. They are all Discovery Studio compatible. All the products you mentioned are still supported.

WAW: But is Accelrys not losing the branding advantage of the famous names behind some of these methods?

FKB: We still talk to customers about the Ludi component and the Catalyst component and these programs still run exactly as they did before.

WAW: Is Accelrys a modeling company?

MJE: Sixty percent of Accelrys' business is still in modeling products such as Discovery Studio and Materials Studio (it used to be 100%). However, our platform and informatics offerings are growing at a 40% rate and obviously becoming a larger portion of the Accelrys' revenue stream. We are also moving upstream into areas such as early development, clinical and even manufacturing with the SciTegic platform as it evolves into an enterprise framework. The modeling market has declined 40% over the last four years. Once we completed the modernization and integration of the modeling solutions we realized it would not generate the type of growth we desire. We began over 18 months ago to develop a much bolder and grander vision for the company surrounding the platform. The modeling codes remain a very important part of that strategy and we will continue to invest and innovate in the modeling and simulation business.

WAW: How many of your R&D staff are working on "science" (for example, 3D pharmacophores and docking solutions), how many on "chemical information" (the Accord product line) and how many on Pipeline Pilot?

FKB: Matrix management makes it difficult to assign precise numbers: many people work on more than one product line. We have not shifted numbers away from modeling. It is hard to say how many people work on Accord now it is componentized, but out of more than 100 in R&D, more than 25, maybe even 40, work on modeling and simulation, and 15 or so on informatics. The 45 remaining staff are in QA

and documentation, shared services, platform integration and interface.

WAW: Who develops new science: you or your partners?

FKB: Both. It's the same as it has always been: some comes from academia and some is written here. We will continue to develop some of our own algorithms, but why reinvent the wheel? We want to work in green fields and on line extensions. One of the strengths of our platform is that we can take a product from an academic group and make it ready for the market in only 3-6 months time. This capability is unique to Accelrys.

WAW: Give me a "green fields" example.

FKB: Biological registration.

WAW: Yes, I noticed that you have a collaborative development agreement with three major pharmaceutical companies to create a biological registration solution. Is a "collaborative development" different from a consortium?

FKB: There are fewer members in a collaborative development and there are opt-out clauses. There is an onus on us to produce. Payments are graduated: costs increase as we deliver. But we haven't given up on consortia. Consortia make sense for nanotechnology, for example. Consortia can be open-ended.

WAW: In general, are you aiming at computational chemists or bench chemists?

FKB: Discovery Studio is for professionals. DS Chemistry, a new product (out soon—maybe) will be aimed at bench chemists. This will be a lightweight version of Discovery Studio for non-modelers. Our interface is very easy to reconfigure. We could strip it down for the chemist. Pipeline Pilot is becoming much more interactive with Ajax on the backend. Ajax is fast and powerful (DIVA-like).

WAW: What advances do you plan in the actual science, as opposed to the methods of delivery or user interfaces?

FKB: We are continuing to drive the science forward. We have improved the performance of the fixed dockers and now we have flexible protein docking and QM/MM. QM/MM is being tested in collaboration with a handful of customers and is available in the DS 2.1 release. A large pharma has submitted an article on our fragment-based docking. We will bring forward these advances in a solution-oriented way. No other company is bringing out new high quality science as quickly as Accelrys.

WAW: One computational chemist tells me that now you have "disemboweled the science into modules

- and widgets” it is hard for him to know what minimizer, or molecular dynamics or homology modeling is hidden behind the widget. Researchers thus do not know how to evaluate the modules or compare them with past experience, he claims.
- FKB: You can do lots of Catalyst operations within Pipeline Pilot. Yes, it’s different but it’s a more user-friendly and more flexible environment. Parts of Ludi are available to different programs. Discovery Studio makes these things more usable. You don’t need to start up the whole of Ludi, Catalyst, whatever. The software is much more controllable and you’ll have a better grasp of what it’s doing. You can mix and match. You can now integrate GOLD, for example. Tibco Spotfire is an Accelrys ISV, and Pipeline Pilot and DecisionSite are tightly coupled. This completely configurable science gives you incredible power. You don’t just think in the box.
- WAW: How can users compare the function of a custom string of CHARMM widgets in Pipeline Pilot with the results from CHARMM itself? How can they validate or verify calculations that are from a custom protocol of strung-together widgets, whose results will depend on the underlying Pipeline Pilot infrastructure and data transfer?
- FKB: Both ways of using CHARMM return the same score results. You can still run CHARMM scripts directly from a command line but there will be no difference from your “widget” version: CHARMM is still the one executable. The results are reproducible.
- WAW: How is all this to be priced? By each widget, or by packages of widgets? How much is a minimizer from CHARMM worth? Is it worth more or less in a package? How will researchers be able to compare packages?
- FKB: Pricing is a competitive advantage and I don’t want to discuss it here but I *can* say that we are creating new pricing models. We want to make sure that customers get what they pay for; we want to produce a packaging that gives everyone an option, an appropriate level of packaging. When you have 50–100 products this is not easy. We’ll have the answer by this summer.
- WAW: Pipeline Pilot is seen as an expensive solution.
- MJE: We have heard the message about pricing. The key words in our approach going forward are “keep it simple” and “price based upon value given to the customer”. In modeling and simulation for example, we will give access to the entire library of code instead of selling individual components, although customers will also be able to buy individual solutions from the library if they desire. The new pricing strategy will be launched in July. It’s all about *value*. You shouldn’t look at the *price* of the software you are using; you should look at the value it is delivering. If you don’t value it, then get rid of it.
- FKB: If you see Pipeline Pilot as a personal productivity tool it will seem expensive. We are talking here about the first-in cost. The technology is shareable. You can use it in preclinical. You can use it in tox. It is integratable and shareable. Once you look at it in that light, it is not expensive.
- WAW: Pipeline Pilot now faces considerable competition from KNIME, and other solutions. How will Accelrys respond to the new market dynamics?
- FKB: Pipeline Pilot is scalable and its data models are better. It has security. It has many more pre-built applications. It is interactive. It has components for R-stats and gene expression and lots of other things and you don’t have to be very expert to implement Perl Scripts. No doubt KNIME will make some headway. You have a case of buy *versus* build here. Using KNIME is like building Pipeline Pilot. These people have actually verified our approach. Incidentally, KNIME components will play in Pipeline Pilot.
- MJE: I agree [with Wendy] that offering Pipeline Pilot free to academics [SciTegic Pipeline Pilot Student Edition] was a move to counter KNIME but we do not have just a platform: we have both our science and our platform. Thirty-seven companies ride on our ecosystem. We are adding major players on a continuous basis, most recently Microsoft and Agilent. So as we continue to amass computing capability on the platform it becomes even more differentiated.
- WAW: For MDL customers considering migration to Isentris, you offer a continuum of solutions, from tools and components through to an out-of-the-box application suite (Accord Enterprise Informatics). This is a very competitive market, dominated (at least until recently) by MDL. Even if Accelrys were to steal a slice of the pie, is the pie big enough to justify your efforts?
- FKB: SciTegic Enterprise Server is a *platform*. It is a software environment and the question is what we build on top. At the moment we offer registration, gene expression, plate management etc. The focus is still R&D but we are moving more toward “D”. Accord Enterprise Informatics is different from the SciTegic Enterprise Server: it addresses *information* more. There is still a

slice of the pie for Accelrys. Pfizer and our other big customers are now using components in SOA strategies: the information, the platform, and the science configurable all together. Some companies such as Schrödinger focus on science but have no informatics. Accelrys has the complete solution.

MJE: Our platform is not a Symyx Isentris competitor. Isentris is a cheminformatics-only play (together with an ELN). Isentris is too monolithic and closed, from my perspective. We have a more open, more widely applicable solution.

WAW: I don't see anything on your Web site about an ELN, although you are reselling Agilent's Kalabie ELN.

FKB: We are agnostic when it comes to notebooks. Yes, we have a partnership with Agilent but, looking forward, we will offer a biological ELN.

WAW: Frank, I'm told that you are into wikis and blogs. Do you think that social software tools are relevant to computational chemists?

MJE: It is interesting that you should ask that because just today [April 21] we have put out a press release about a collaboration to support scientific applications through Microsoft Office SharePoint Server 2007. This will allow us to deliver scientific capabilities and content to the broader scientific community *via* their desktops. Microsoft's broad reach further enhances the Accelrys ecosystem and expands our market opportunity as it helps us to deploy leading-edge technology that will enable rich scientific collaboration and allow research teams to make more informed decisions.

WAW: Mark, Accelrys has not shown a profit recently and your stock price has also declined steadily since early December. It is nearly time for you to release results for the last financial year. Are things going to get any better?

MJE: At our last earnings call [January 2008] we predicted continued order intake growth in Q4 following order intake growth in Q3. Keep in mind our financial year ended in March 2008. Last year, in 2007 (our fiscal 2008), we actually produced a \$4.8 million NON GAP operating profit and \$5 million in added cash flow. The SEC in the US changed the accounting laws during the year so you have to expense stock options, thus creating the difference with GAP earnings. Note that our cash increase matches the profit. At one time this company was losing \$15–20 million a year and burning an equal amount of cash. Last year it generated \$5 million cash. As it relates to the stock, I believe we are

significantly undervalued, partly due to the microcap status and the current economic conditions. Also, we have not proven to the street that we can grow yet. I am confident in time all will be in balance.

WAW: Why did you close your Bangalore R&D facility?

MJE: I took over at Accelrys five years ago. It was my choice to set up the R&D department in Bangalore and I had done it in a previous company with much success: I saw it as one of the necessary avenues we had to take to modernizing and reversing the \$20 million loss. The Bangalore strategy worked while we were in the integration and modernization phase, while we were bringing everything together. Out of 75 employees in Bangalore, more than two thirds were in QC. After two to three years, the modernization phase was over. Building code over there was a challenge. Not only are the science problems we face complex but we had to face up to wage inflation in India and rapid staff turnover. We want to work side by side with our customers and the time zone and cultural differences were an impediment.

WAW: What have you to say to disappointed users of GCG, which is no longer being developed and will no longer be offered after June 2008?

MJE: We cannot continue to support GCG. So much software of that type is now open source. We have explored all sorts of options to keep GCG going but we can no longer invest in this. We do have a free SciTegic platform for academics, and select bioinformatics functionality is available for both Discovery Studio and Pipeline Pilot.

WAW: To what extent are you reviving the company's prospects by cost-cutting? I noticed, for example, that you had a rather low key booth at the ACS meeting in New Orleans and you are no longer sponsoring the ACS award for computers in chemical and pharmaceutical research.

MJE: We have made some cutback on costs: for example, years ago we had over 700 employees, now we have 380, which is the appropriate amount for our size. Investment in science and customer contact remains a top priority. As it relates to our future prospects I believe we have stabilized the modeling and simulation business. As I mentioned earlier the platform and informatics solutions are growing nicely. In fact I can now state that all twenty of the top pharma companies use our platform. In one of those companies there are over 1500 employees engaging with the platform on a consistent basis.

WAW: Mark, would you like to sum up your vision?

MJE: We are a company delivering solutions across the entire continuum of discovery, development and manufacturing with the platform being the integration backbone on which solutions are delivered. We are continuing to invest in new releases of our modeling software, but we are investing at a greater pace in platform and informatics; one example is the imaging analytics collection we just brought to market. We have built our platform and solutions based on a service oriented architecture and we have a massive ecosystem of software suppliers and competitors: large companies like Agilent, Microsoft etc. working on the platform. In most cases our customers have forced our competitors to join our ISV program. We are a company with a big vision that is no longer just about modeling and simulation but providing solutions that increase productivity and help our customers along the entire continuum to make informed, real time decisions. In essence, we inhale data from disparate sources, manipulate it through advanced analytics of which our predictive modeling and simulation codes are part (and our ecosystem) and then report the data in numerous ways from static reports and interactive visualization to advanced three-dimensional viewing. Our customers build protocols and automate their workflows using our technology. Maybe it is trite to say, but we actually turn data into insight or knowledge for our customers.

## Comments

Modeling has never been a big market and it is not getting any bigger. Delivering the old point solutions offers little scope for growth and one by one the modeling and cheminformatics companies are having to re-invent themselves. Accelrys is no exception, and being the biggest of a

select group, it had either the most to gain or the furthest to fall. It also has the greatest complexity—a very large number of software brands across both materials and life sciences—but the variety does give Accelrys scope for expanding across “the continuum”.

It seems no time at all since “axle grease” was hailed and now we have another re-invention. Early in 2007 press releases told us that “Accelrys has over twenty years of innovation and technology leadership in delivering software and service solutions that transform discovery and development research”. By September 2007 the new vision was becoming obvious: “Accelrys develops and commercializes scientific business intelligence software for the integration, mining, analysis, modeling and simulation, management and interactive reporting of scientific data”. Bog standard cheminformatics is old hat now: decision support and business intelligence are the “in words”.

The old hands are going to have to accept that “widgets” are the way forward. Throughout my lengthy discussions with Frank it was clear that he was not just feeding me marketing hype: he really believes in his configurable science theme. Bear in mind, also, that Frank is an “old hand” himself, who knows a thing or two about both science and user-friendliness. He spoke briefly but affectionately about DIVA, which is still available in the Accord suite. It hasn’t changed much in 12 years, since GSK and Oxford Molecular co-developed it. It still has broad audience appeal, he says.

Mark cannot waste time on sentiment. He has had to turn round a \$20 million loss and convince the street that you can make money from “scientific business intelligence”. He has to grasp the nettle when it comes to pricing his “widgets”. My first impression in talking to him was that he must have at least some marketing background. His background is actually finance through and through, but he had a way with words when it came to ecosystems and the continuum, I suppose because, in order to achieve his financial aims, he has to convince the customers and the shareholders (not to mention Wall Street) about his vision. We will have to wait and see whether the vision can be turned into reality after the re-branding in summer 2008.