



# Mathematical Solutions for Applications in Computational Biology

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# Agenda

- Power to Solve Complex Problems
- Computing Language Dynamics
- Leveraging Mathematical Libraries
- Examples
- Academic support: Visual Numerics' Education Programs

# Solving Complex Problems

Significant improvements in compute power over the past five years has spurred the development of complex mathematical models.

# Solving Complex Problems

- Availability
  - Desktop – Prototyping
  - Servers and clusters – run the models
- Accessibility
  - Powerful systems within departments
- Portability
  - issues diminishing
  - 32 bit vs. 64 bit

# Computing Language Dynamics

- **Fortran**
  - Optimal performance for computations
  - Development tool support: compilers; math libraries
  - Portable?
- **C/C++**
  - Flexible
  - Performance improving
  - Improvements in development tool support
- **Java**
  - Performance a consideration
  - Portable: Collaboration and deployment
  - Development tool support: early stages

# Leveraging Math Libraries

## IMSL™ Numerical Libraries

- Focus on the model, not all aspects of the underlying mathematics and statistics
- Reduce the development effort
  - Algorithm development
  - Porting and maintaining source code
- Portability: desktop to server
- Language flexibility
- Reliability

# Examples

- Duke University: Dr. Tom Keppler
  - Immune response to bio-terror threats
  - IMSL™ Fortran Library
  - Diff. Equations, quadrature, statistics
- U. of Alabama-Bghm: Dr. David Allison
  - HDBStat! – Micro-array data analysis
  - JMSL™: Numerical optimization and statistics

# Examples

- Columbia University: Vezen Wu
  - MedfoLink: Forecast disease outbreaks
  - JMSL™: Forecasting, statistical analysis
  - MedfoLink: A Powerful Concept-Based Approach to Medical Reports Processing
- U. of California-Davis: Dr. David Rocke
  - Biostatistics
    - NMR spectroscopic metabolomics data analysis
    - Gene expression analysis
  - Numerical optimization, Generalized Linear Models, Large scale band matrix solvers
  - IMSL™ Fortran Library

# Visual Numerics' Education Programs

- Formed Jan. 1, 2004
- Focus on the use Visual Numerics' technology in the academic community
- Research: Meet the requirements of collaborative research
  - Sharing of applications
  - Incorporate technology into textbooks
  - Application development support on servers and clusters

# Summary

- Computational landscape continues to change (*for the better*)
- Commercially available math libraries must adapt to the changing requirements
  - Languages
  - Research
  - Classroom

# Questions?

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