Utah-Buenos Aires Grid for Chemical Physics: NMR Chemical Shifts, Genetic Algorithms and Growth Pattern Formation in Thin-layer Cells.

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What are Chemical Shifts ?

- Are the “shift” of the NMR signal due to the molecular and crystalline environment.

- Tensorial quantity, i.e. the shifts depends on the orientation of the molecule in the magnetic field.

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Why Chemical Shift Calculations are Important ?

- Chemical shifts are highly dependent of Molecular and Crystalline Structure.
- Chemical Shifts Calculations provide the link between “structure” and “measurements”

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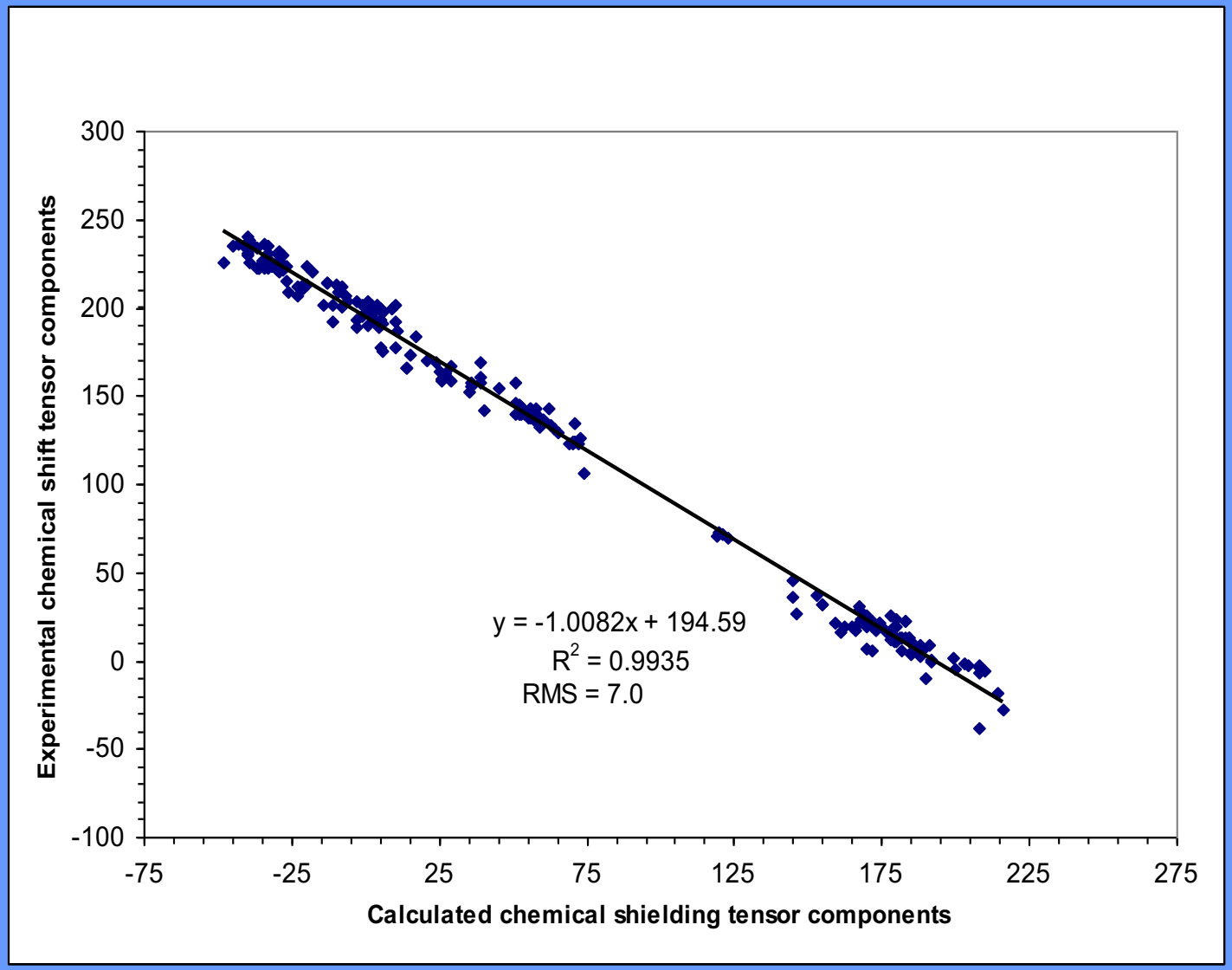

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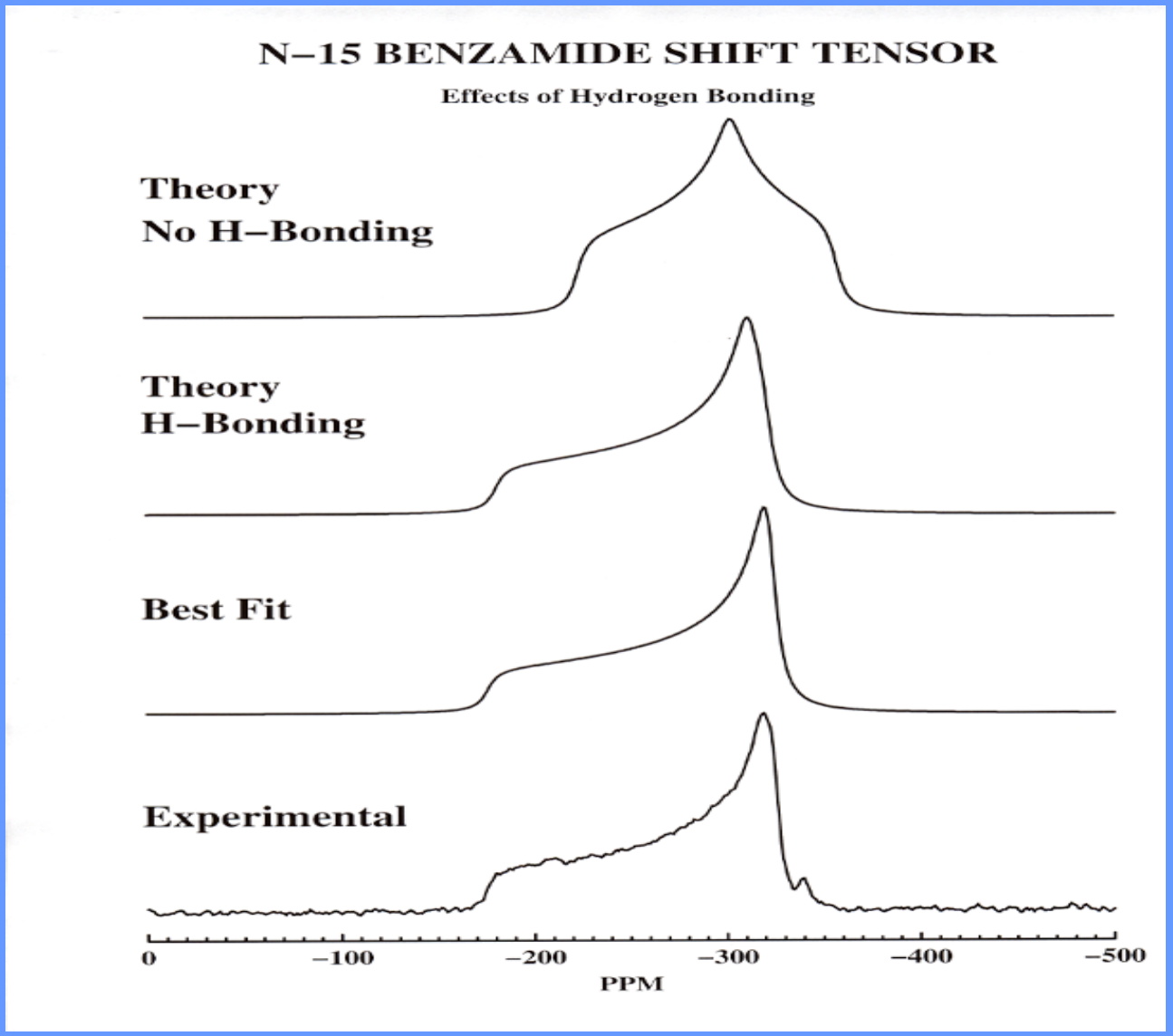

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Genetic Algorithms

- Minimization methods based in the Darwinian principle of survival of the fittest.
- Genetic algorithms can provide not only a global minimum, but also information on other states with energies or properties close to the minimum.
- Genetic Algorithms are amenable to efficient parallelization and Grid computing.

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Modified Genetic Algorithm to Model Crystal Structures

- Proved very effective for rigid molecules.
- It has been modified to use empirical potentials for flexible molecules.
- Will be adapted to use experimental and calculated NMR chemical shifts information in the optimization method.

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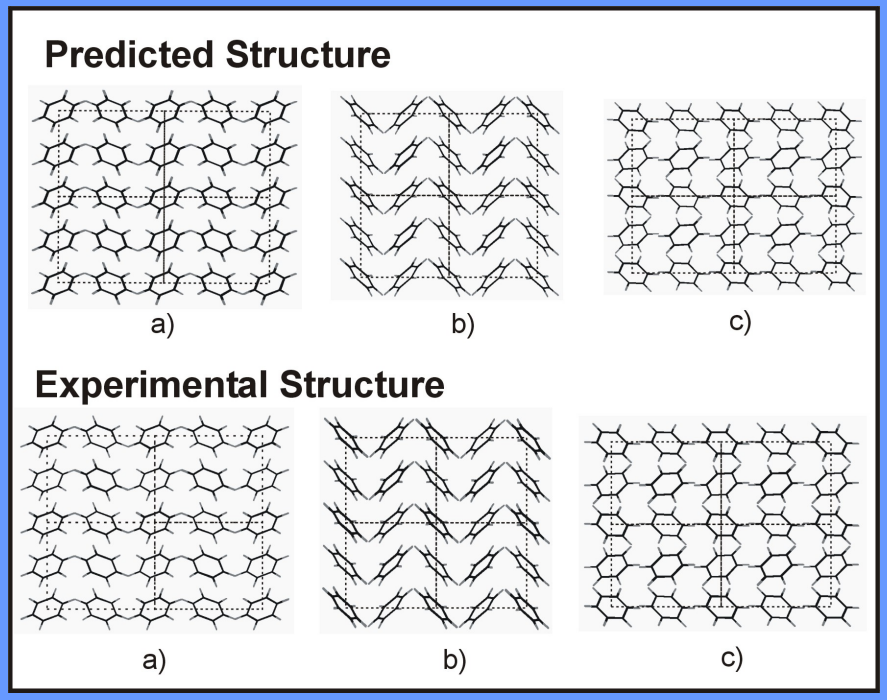
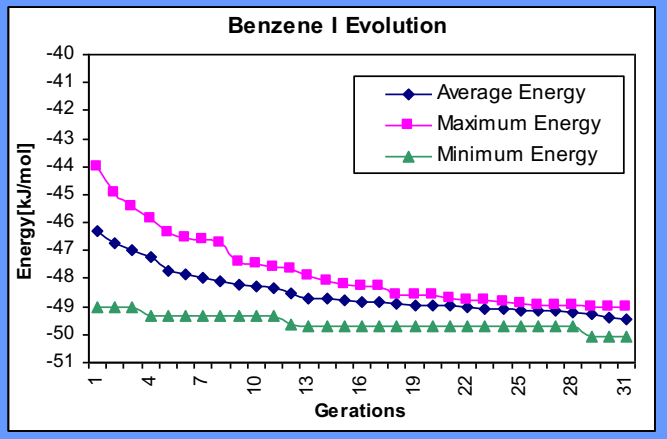
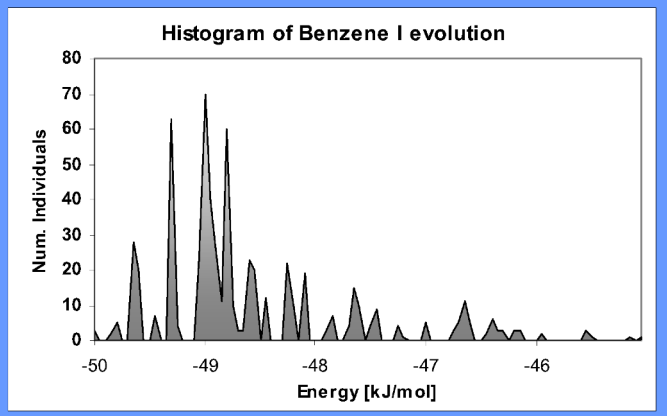
MGAC : Modified Genetic Algorithm for Crystal and Cluster Structures







The code was run on Linux-Cluster with 12/300 nodes.

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Growth Pattern Formation in thin-layer cells

- Growth pattern formation (GPF) is a common phenomenon in a wide range of problems from physics to biology.

- The interpretation of these measurements require numerical simulations of macroscopic model recently developed.

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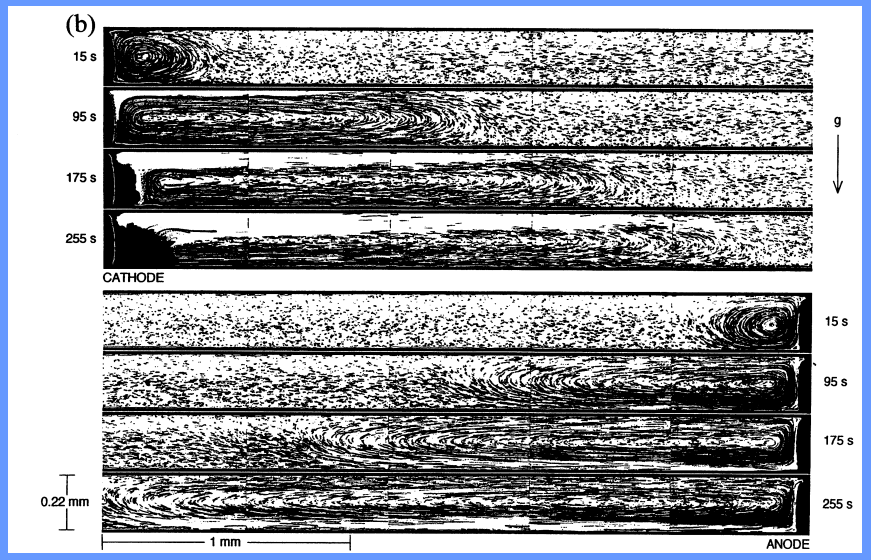

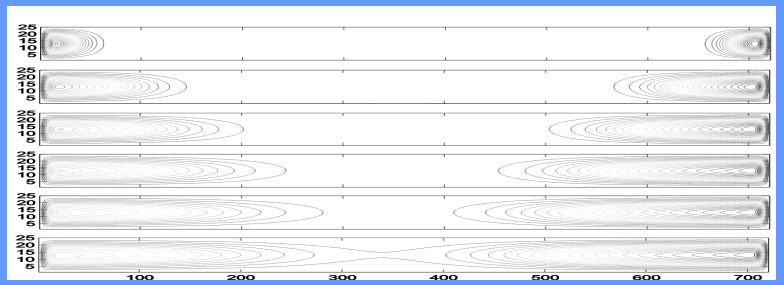

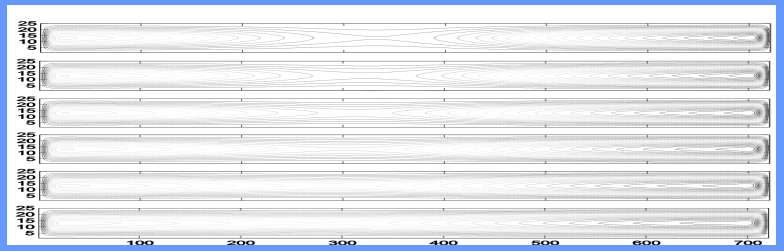

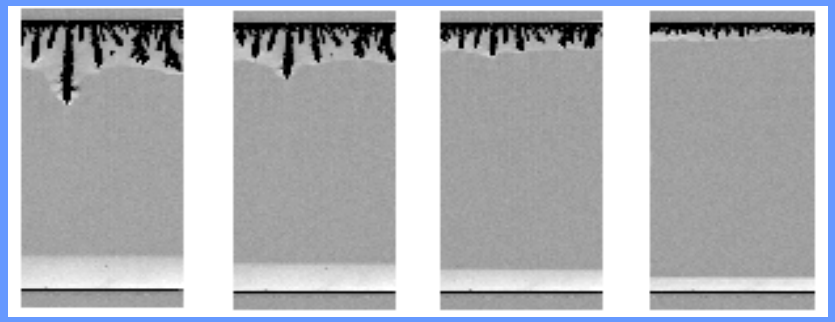

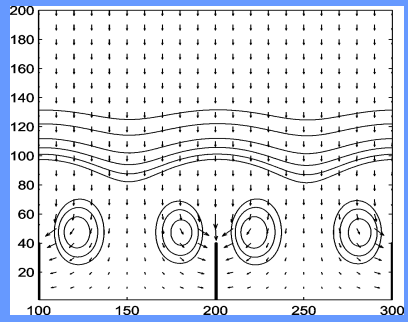

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Objectives of the Collaboration

- Leverage expertise and resources available in Utah and Buenos Aires
- Develop robust computational techniques to allow these compute intensive Chemical Physical applications to take advantage of inter-continental Grid resources.
- Develop an student training program in computational chemical physics with emphasis in Grid Computing.

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Combine resources in the Buenos Aires and Utah groups

- Buenos Aires:
- Theoretical expertise on chemical shifts
- Programing capabilities

- Utah:
- Large computational resources
- Experimental NMR Lab.

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Network Needs

- **End-to-end connectivity from FCEyN to CHPC for:**

- Remote access to systems via Globus like infrastructure.
- Efficient file sharing, including pre-staging.
- Distributed scheduling of processing and data staging.

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Network Needs (cont.)

- I2 type of services from FCEyN to CHPC
  - Teleconferencing,
  - Distributed white boards and
  - Remote instrument operation

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