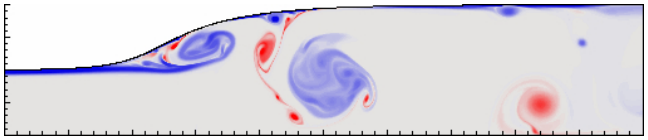
CIMMS

A modeling and analysis framework for systems whose large-scale information is not available

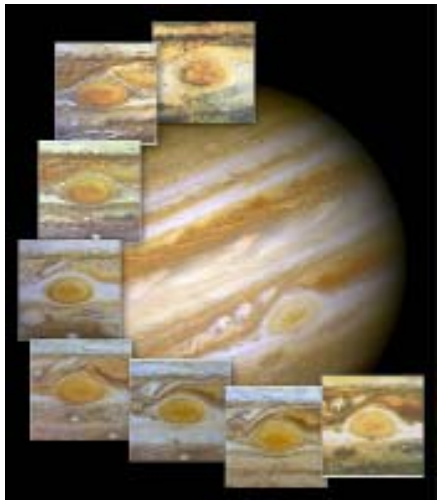


CIMMS lunchtime discussion group
Jimmy Fung, 10 October 2002

Advisors: T. Colonius, R. Murray

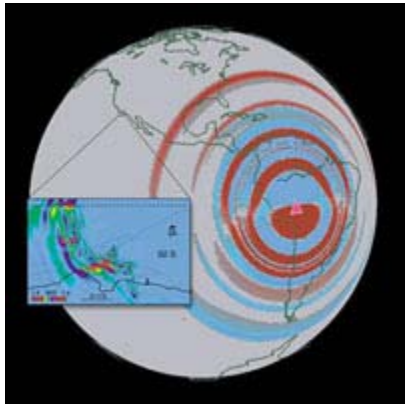
www.cimms.caltech.edu

What is large scale information?



- Bulk, coarse, macroscopic, systems-level, coherent quantities
- "Governing moments"

- Typical systems display:
  - Separation of scales
    - Eigenmodes
    - "healing" of higher-order scales/modes
  - Information management by scale



Big whorls have little whorls which feed on their velocity,
and little whorls have lesser whorls
and
so
on
to
viscosity.

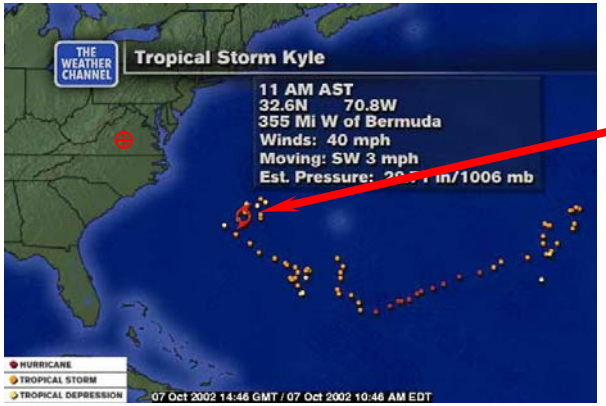
--Lewis Richardson

Extracting large-scale information

- Reduced-order modeling
  - Simplified dynamics models
  - Reduction methods
  - Advantages
    - Direct treatment of large-scale information
    - More immediate access to results
  - Disadvantages
    - Availability / application overhead
- High fidelity experiments
  - Laboratory
  - Numerical
  - Advantages
    - Complete treatment of the phenomena of interest
  - Disadvantages
    - Time and resource constraints
    - Post-processing must be performed to answer large-scale-type questions

a question

- What can we do if reduction procedures and high-fidelity experiments are neither practical nor feasible?



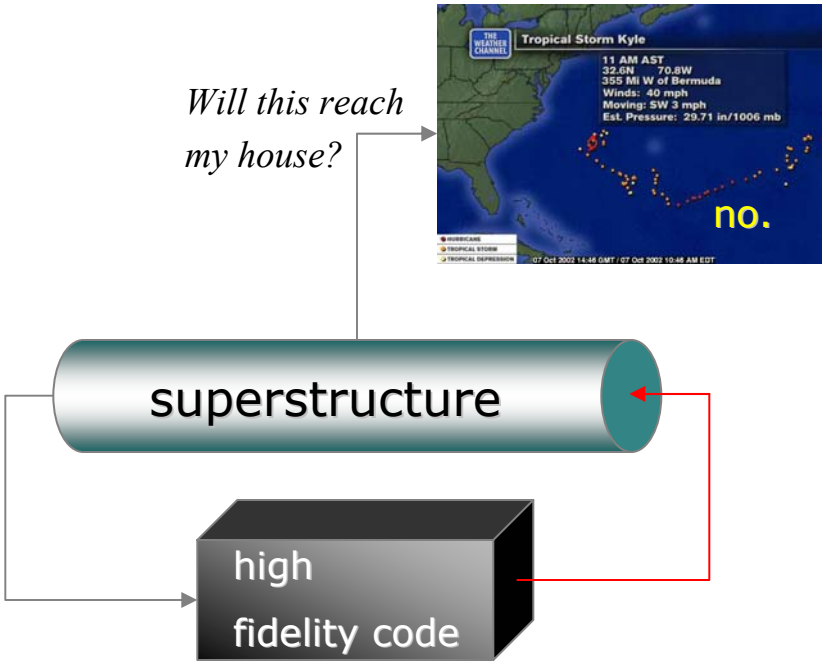
Will this reach my house?

This is a question with the system, or the large-scales, in mind.

For example, suppose we have preexisting code for studying a class of problems, and we encounter something too complex to simulate with the code.

Objective

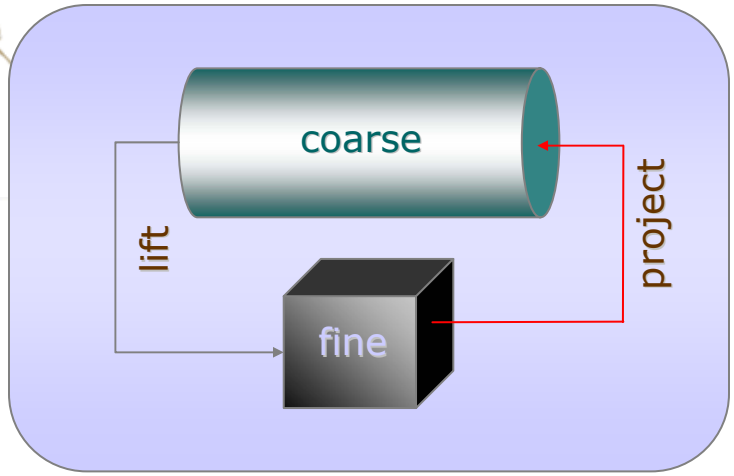
- Answer systems-level questions when
  - The system may admit to reduction (which is not easily implemented)
  - High-fidelity tools are available (although information management is not desirable or practical)
  - We want to address (manage) large-scale information directly

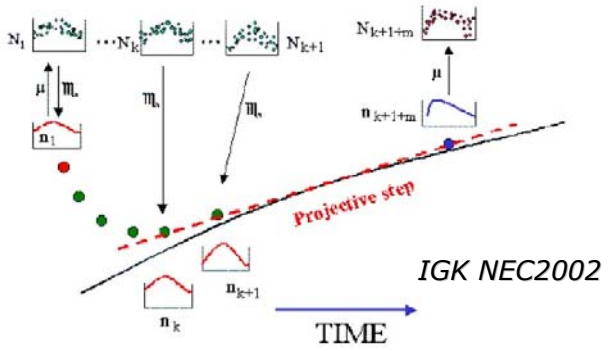


Use existing high-fidelity tools, with a computational superstructure, to approximate the reduction and answer systems-level questions.

Temporal coarse analysis

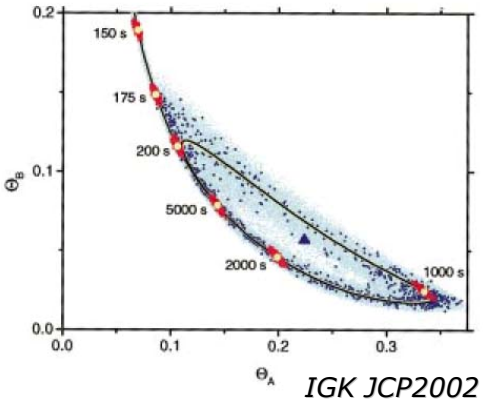
ref:// I. G. Kevrekidis





IGK NEC2002

- The coarse (large-scale) time-stepper
  - Define the coarse initial condition.
  - Lift to consistent fine (high-fidelity) initial conditions.
  - Evolve using the high-fidelity simulator.
  - Restrict and project the coarse state to future times.

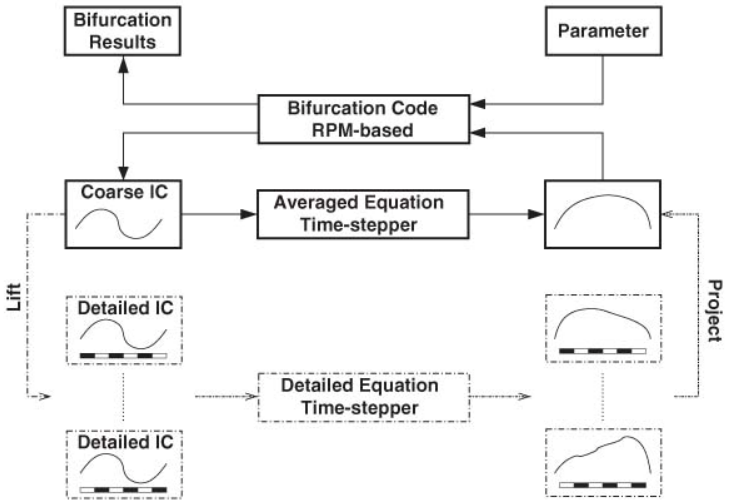


IGK JCP2002

Temporal coarse analysis

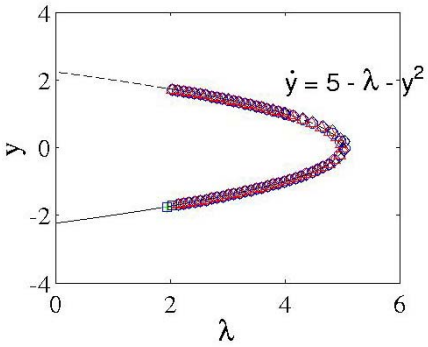
ref:// I. G. Kevrekidis

- Coarse bifurcation analysis
  - Additional superstructure wrapped around the coarse time-stepper



IGK Nonlinearity2002

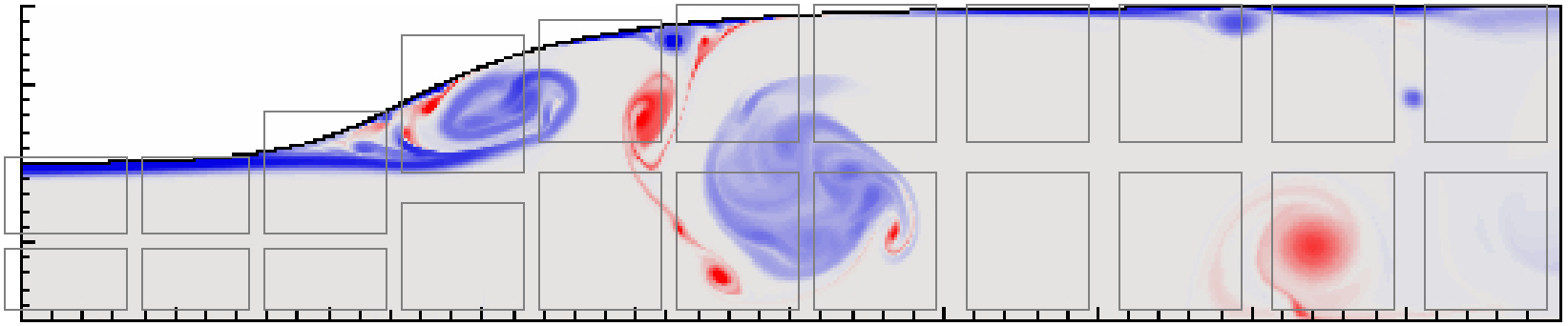
pseudo-arclength RPM



Spatial coarse analysis

ref:// I. G. Kevrekidis

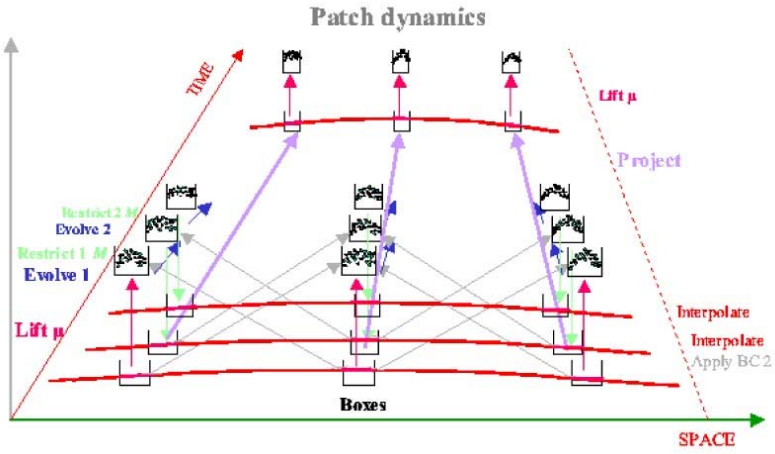
- The gaptooth scheme for evolution on a coarse grid
  - Similar to the coarse time-stepper
  - The lifting operators now include treatments for boundary conditions and initial data



Spatio-temporal coarse analysis

ref:// I. G. Kevrekidis

- Patch dynamics
- Patch boundary / initial conditions

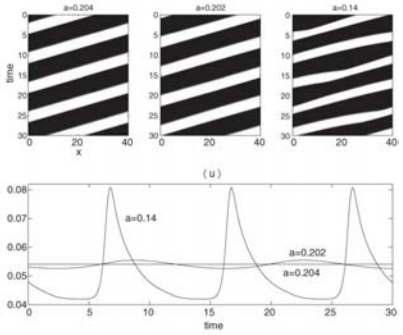


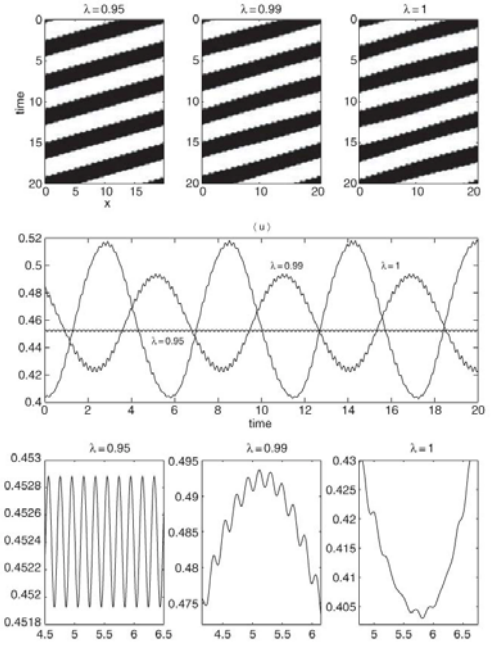
IGK NEC2002

Reaction-diffusion system [Kev]

ref:// I. G. Kevrekidis

- Microstructured composite catalysts
  - CO oxidation over a composite medium



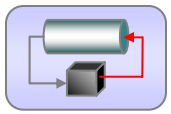


$$u_t = u_{xx} + \frac{1}{\varepsilon} u(1-u)\left(u - \frac{w + b(x)}{a(x)} \right)$$

$$w_t = g(u) - w$$

Bifurcation from a steady pulse to a modulated breathing pulse

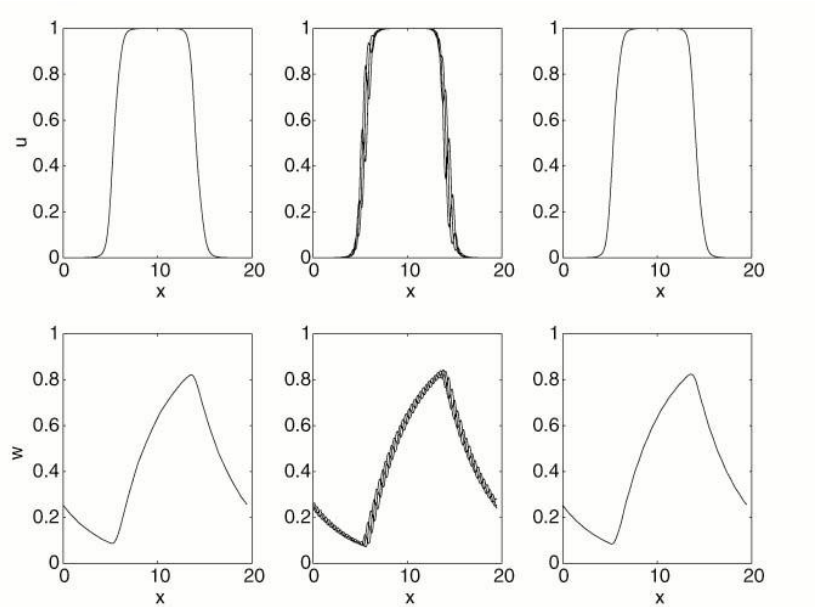
IGK Nonlinearity2002

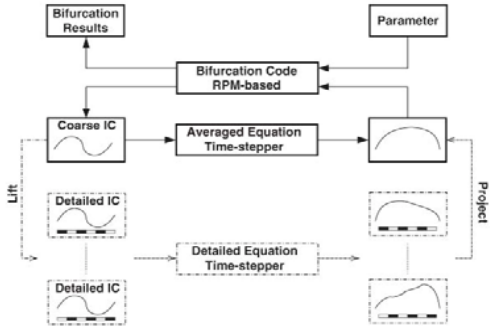


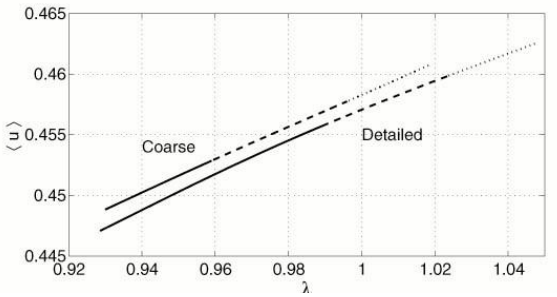
Reaction-diffusion system [Kev]

ref:// I. G. Kevrekidis

- Coarse bifurcation solution



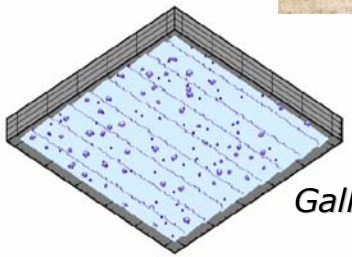




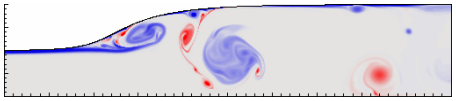
IGK Nonlinearity2002

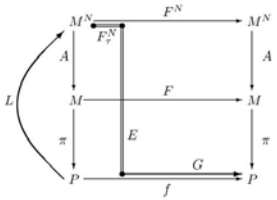
Future directions

- Applications
  - Turbulence
  - Quantum-classical limit
  - Control system development
    - Thin film growth
  - Systems applications
- Current work
  - Diffuser performance
  - Mathematical description



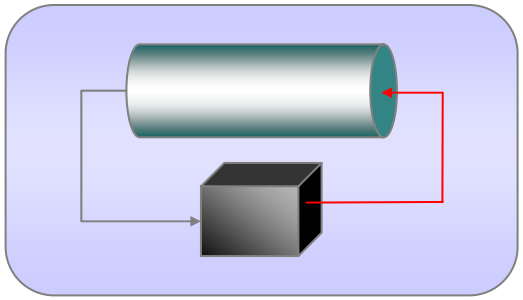
Gallivan

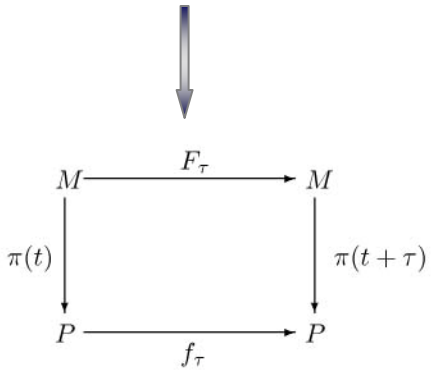




Black-box, computer-assisted analysis

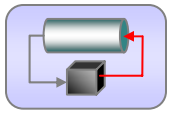
Mathematical description





- Purpose and utility
  - Error estimation
  - Robustness

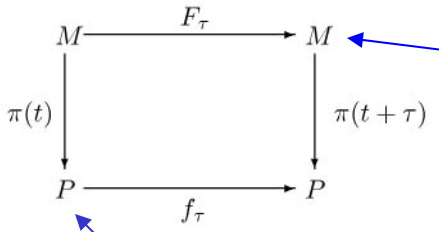
Construction of new computer-assisted analysis tools



CIMMS

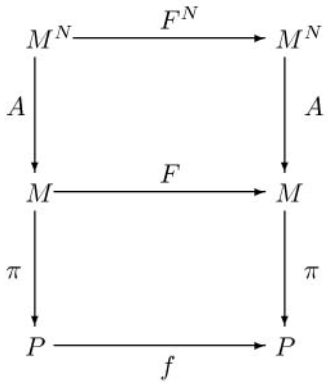
Mathematical description

work in progress



fine

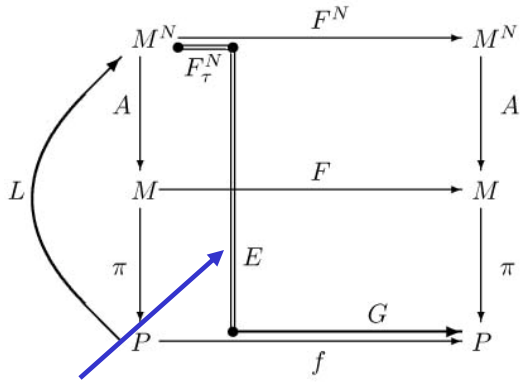
coarse



questions

$\pi \circ f = F \circ \pi$?

What if f is not available?

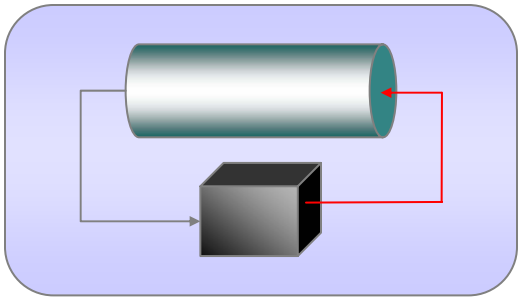


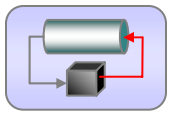
lift

project

Concluding remarks

- Computer-assisted analysis tools are on the horizon
- These tools complement traditional reduction and simulation techniques





References

- Acknowledgements: R. Murray, T. Colonius, J. Marsden, C. Rowley, IGK

- I. G. Kevrekidis
  - "Coarse Stability and Bifurcation Analysis Using Stochastic Simulators: Kinetic Monty Carlo Examples.", *J. Chem. Phys*. 116(23), 2002, 10083-10091. With Alexei G. Makeev et al.
  - "Effective Bifurcation Analysis: A Time-stepper Based Approach", *Nonlinearity* 15, May 2002, 491-571. With Olof Runborg et al.
  - "Equation-Free Multiscale Computation: enabling microscopic simulators to perform system-level tasks", *NEC*, 2002. With C. William Gear et al.