Algorithmic Development for Informative and Intelligent Scientific Computation

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A word about CM3

Computational Mathematics and Multiscale Modeling (CM^3)

CM3 collaborates with various groups in Columbia: APAM/CS/CEEM/MECH, DSI, and Law School,...

Recent funded projects @CM3

- 2020-23 NSF-DMS: Numerical analysis of asymptotically compatible discretization of nonlocal models.
- 2020-21 AWS ML award: Multi-autonomous vehicle driving policy learning for efficient & safe traffic
- 2020-25 NSF-DMS: Research Training in Applied Mathematics at Columbia University
- 2019-23 NSF-DMREF: Complex nanofeatures in crystals: theory and experiment meet in the cloud
- 2017-20 NSF DMS: Numerical analysis of SPH type methods via nonlocal models
- 2017-20 NSF CCF (TRIPODS): From foundations to practice of data science and back
- 2015-19 NSF-DMREF: Deblurring our view of atomic arrangements in complex materials
- 2015-17 DARPA EQUiPS: Foundations of rigorous mathematics for UQ in large systems at extreme scale
- 2015-22 ARO-MURI: Fractional PDEs for conservation laws and beyond: theory, numerics & applications
- 2015-16 AFRL-STTR: Data infrastructure for materials genome with innovation and certification
- 2013-19 AFOSR-MURI center for Material Failure Prediction through Peridynamics

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** Jointly with collaborators from other institutions and/or national labs.

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Reflecting the theme of **informative and intelligent scientific computing**.

Paradigm shift of scientific computing over the years:

- **O-O**: Operational and Optimized

  (executable, efficient, ...)

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- **V-V**: Validated and Verified

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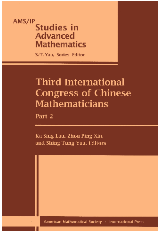
- **I - I**: Informative and Intelligient

  (smart algorithms, knowledge extraction/discovery, ...)



Informative and intelligent scientific computing
(Du: ICCM2004, published 2008, 731-748)

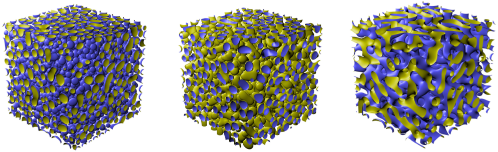
Algorithmic development for traditional scientific computing

- Operational & Optimized, physics/model-based simulations, from Tera, Peta, to Exa-scale, ...

[1] J.Zhang-C.Zhou-Y.Wang-L.Ju-Q.Du-X.Chi-D.Xu-D.Chen-Y.Liu-Z.Liu, SC16, IEEE 2016

Algorithmic development for traditional scientific computing

- Operational & Optimized, physics/model-based simulations, from Tera, Peta, to Exa-scale, ...
- Eg. *Record-breaking* phase field simulations of microstructure evolution, from nucleation to coarsening, at extreme-scale for Gordon-Bell competition: with peak over 50 PFlops, 21.5 trillion Grid-Points, 10 million Processing-Elements.



(3D microstructure evolution involving complex topological changes[1])

- Algorithmic development: high order discretization, localization, domain decomposition ⇒ **scalable**

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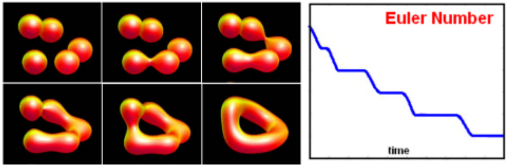
Algorithmic development for informative and intelligent scientific computing

Keys for I^{2}SC: extracting hidden information, learning from simulation/data, smart computing.

Illustrative examples (from the past):

- Extracting hidden topology of simulated microstructure with implicitly represented interfaces



Reverse thinking:

algorithms for computing Euler number to learn/detect topology change (Du et al 2005)

- CAMLET (Combined Ab-initio and Manifold LEarning Toolbox): NSF-CCF (CS/Math/Phys/Stat) 2004-07; smart computing with surrogate models learned from database of ab-initio simulations.

- Shrinking dimer dynamics (SDD) + KMC for transition state search and nucleation/coarsening.

Algorithmic development for informative and intelligent scientific computing

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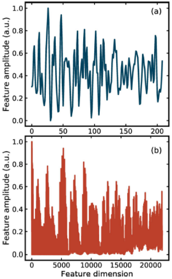
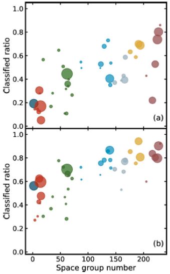
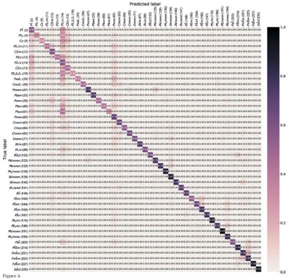
Illustrative examples (more recent ones):

- Nanostructure inverse problem (NSF-DMREF, with Billinge group, 2015-).

  Extracting materials structure information from x-ray data (PDF) with optimization and deep learning. E.g. group symmetry classification using CNN. (Liu et. al. 2019, Acta Crys. A)







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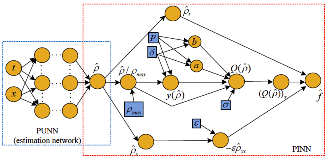
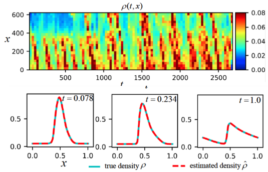
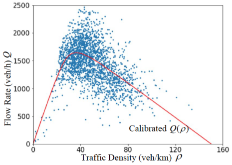
Illustrative examples (more recent ones):

- Physics-informed deep learning of traffic state estimation (with X. Di of CEEM Shi et al, 2020)







- Autonomous experiment design with meta-modeling and machine learning:
  - exploring structure-synthesis-property relation for materials discovery,
  - cooperative and non-cooperative games and reinforcement learning for constitutive modeling, (e.g., work with S. Sun group of CEEM, Wang et. al. 2020).

Physics-based and data-driven modeling and simulations

Advent of computing technology

$+$

Access to large amount data

$+$

Improved machine learning

$\Downarrow$

Physics-based/data-driven modeling

$\Rightarrow$ Capturing the essence of I^2SC:

Iteratively solve forward+inverse problems.

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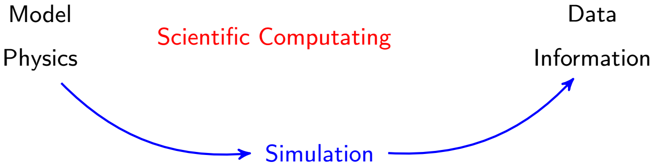

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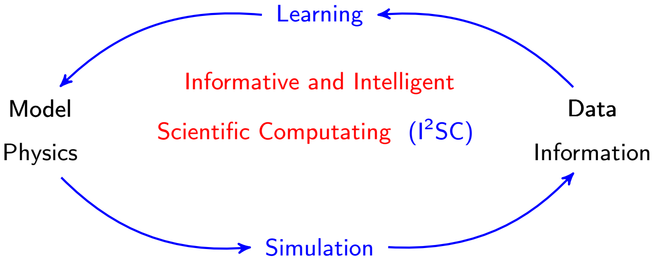

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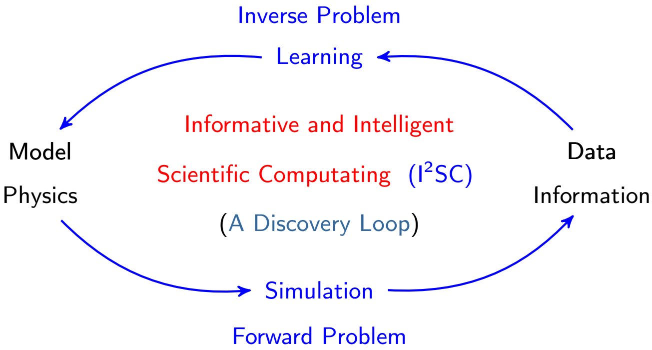
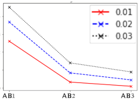


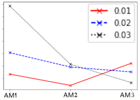
Informative and Intelligent Scientific Computing (I^2SC): Forward + Inverse

Eg: Integrating given dynamics (forward) and learning unknown dynamics (inverse).

⋆ Learning/predicting dynamics from video sequences (jointly with Hod Lipson group)

⋆ Numerical integrator: good (stable) for given dynamics $\neq$ good for dynamics discovery.





New stability/consistent theory for learning with LMMs (2020)

I^2SC $\Leftrightarrow$ computing and learning $\Leftrightarrow$ knowledge discovery (robust/predictive/trustworthy/automated)

Learning$\neq$black box $\Rightarrow$ new challenges to algorithmic development: adaptive/multiscale computation, error/uncertainty quantification, dimension reduction (thus modeling nonlocal interactions), ...

Thank you!