Large-scale simulations of complex physical systems

Aleksandar Belić,
Scientific Computing Laboratory
Institute of Physics
Belgrade, Serbia

April 21, 2011

Scientific Computing Laboratory (www.scl.rs)

People

- Researchers: A. Belic, D. Arsenovic, A. Balaz, A. Bogojevic, N. Buric, M. Milovanovic, I. Stankovic, D. Tanaskovic, S. Vrhovac, N. Vukmirovic
- Students: M. Radonjic, J. Scepanovic, V. Slavnic, D. Stojiljkovic, I. Vidanovic, J. Vucicevic, D. Vudragovic, M. Zezelj
- Staff: B. Ackovic, N. Grkic, I. Smolic

Infrastructure

- PARADOX: ~1000 cores parallel cluster, major upgrade expected
- 10 Gbps dedicated link

Research program

- Basic research
  - Efficient calculation of path integrals with applications to ultra-cold quantum gases
  - Modeling and simulations of granular materials
  - Study of strongly correlated quantum systems
  - Modeling of information processing in complex classical and quantum systems
  - Modeling of transport processes in nano-structured materials and organic semiconductors
- Applied research
  - Cluster integration & monitoring tools (GRID, HPC)
  - Engineering simulations

Projects

- National: ON171017, AEGIS (III43007, III45018)
- FP7: PRACE-1IP, HP-SEE, EGI-Inspire
- Bilateral: CH, DE

SCIENTIFIC COMPUTING LABORATORY

April 21, 2011

Simulation – new heuristic tool

- Simulations are modifying the scientific method
- They are neither experiment (input is ours) nor theory (output unknown, its being “measured”)
- Closest definition: new heuristic tool (heuristic ≡ leading to a new knowledge)
  - Usage:
    - Solving analytically untractable mathematical models
    - Numerical solution leads to better understanding of a phenomenon and to establishing a “phenomenological” laws (for a model)
    - New analytic input leads to improved model and/or algorithm, which leads to further insights, ...
    - Uncontrollable escalation in our understanding
- How big is simulation “market share”?
  - Conservative estimate for physics in 2000: >10%
  - realistic estimate today: 25% and growing

Granular materials (1)

Large conglomerates of macroscopic inelastic particles

Applications: Mining, Agriculture, Civil engineering, Chemical, Pharmaceutical...

Goals

- construct statistical and fluid descriptions of cooperative phenomena in the dynamics of powders
- study relationship between the macroscopic behaviour of granular materials and their microstructures

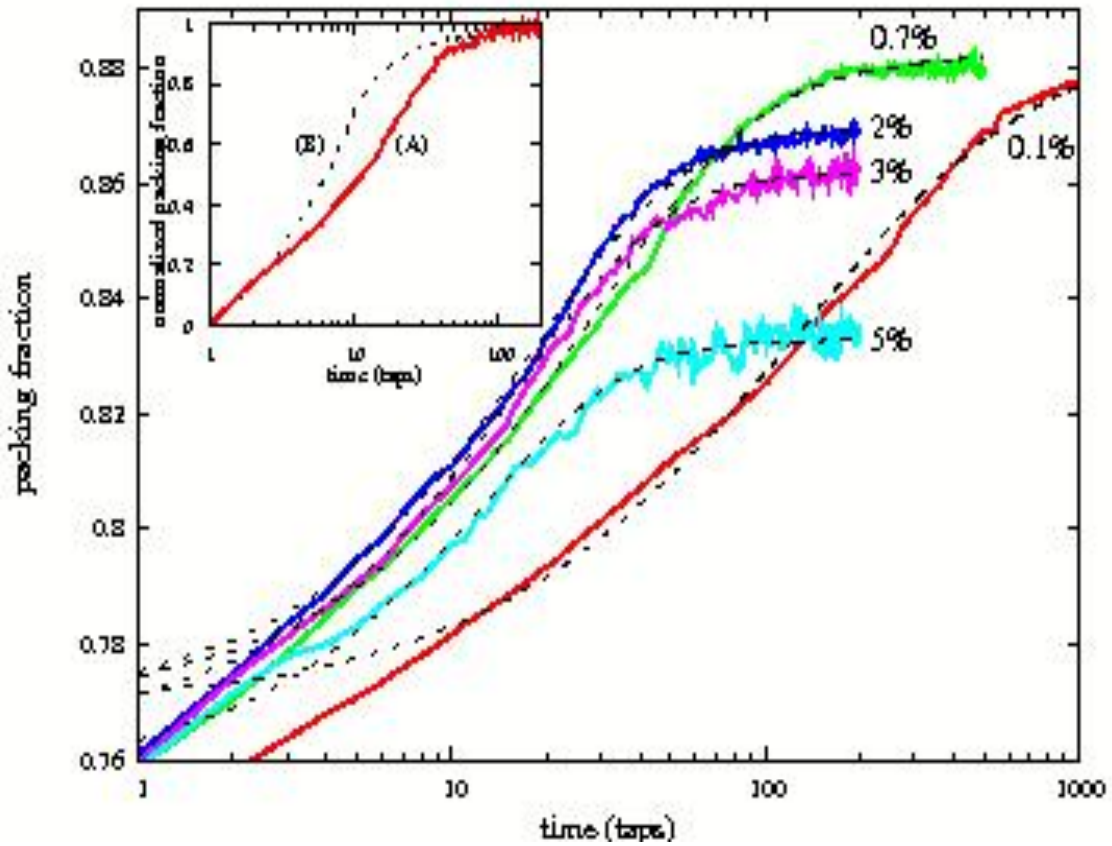
Recent results

- S. B. Vrhovac, D. Arsenovic, and A. Belic, *Phys. Rev. E* **66**, 051302 (2002).
- S. B. Vrhovac and Z. M. Jaksic, *J. Stat. Mech.,* P06008 (2004).
- Lj. Budinski-Petkovic, M. Petkovic, Z. M. Jaksic, and S. B. Vrhovac, *Phys. Rev. E* **72**, 046118 (2005).
- Lj. Budinski-Petkovic, and S. B. Vrhovac, *Eur. Phys. J. E* **16**, 89 (2005).
- S. B. Vrhovac, Z. M. Jaksic, Lj. Budinski-Petkovic and A. Belic, *Eur. Phys. J. B.* **53,** 225 – 232 (2006).
- D. Arsenovic, S. B. Vrhovac, Z. M. Jaksic, Lj. Budinski-Petkovic and A. Belic, *Phys. Rev. E* **74,** 061302 (2006).
- I. Loncarevic, Lj. Budinski-Petkovic and S. B. Vrhovac, *Eur. Phys. J. E.* **24,** 19 – 26 (2007).
- I. Loncarevic, Lj. Budinski-Petkovic and S. B. Vrhovac, *Phys. Rev. E* **76,** 031104 (2007).
- Lj. Budinski-Petkovic, I. Loncarevic and S. B. Vrhovac, *Phys. Rev. E* **78,** 061603 (2008).
- I. Loncarevic, Lj. Budinski-Petkovic, S. B. Vrhovac and A. Belic, *Phys. Rev. E* **80,** 021115 (2009).
- I. Loncarevic, Z. M. Jaksic, S. B. Vrhovac and Lj. Budinski-Petkovic, *Eur. Phys. J. B.* **73,** 439 (2010).
- I. Loncarevic, Lj. Budinski-Petkovic, S. B. Vrhovac and A. Belic, *J. Stat. Mech.,* P02022 (2010).

SCIENTIFIC COMPUTING LABORATORY

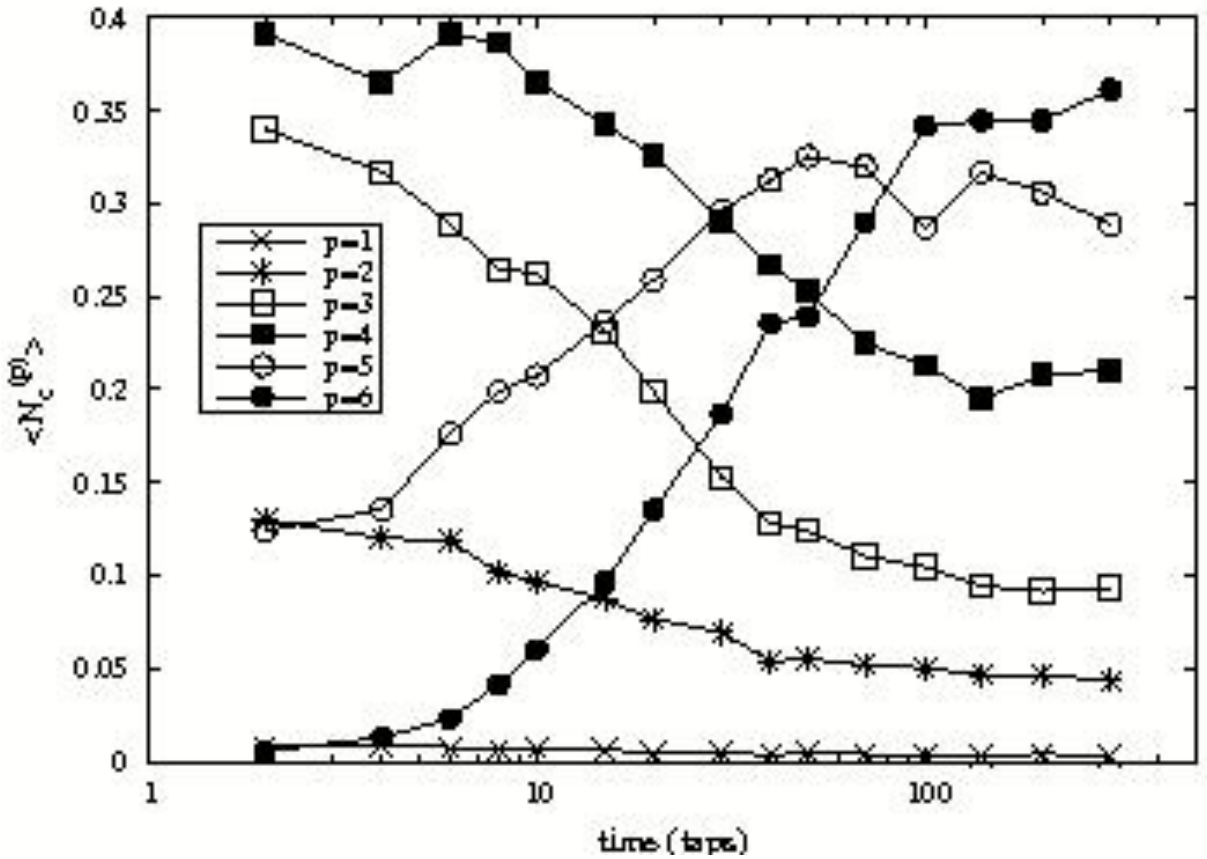
Granular materials (2)

- Time evolution of the density during the compaction



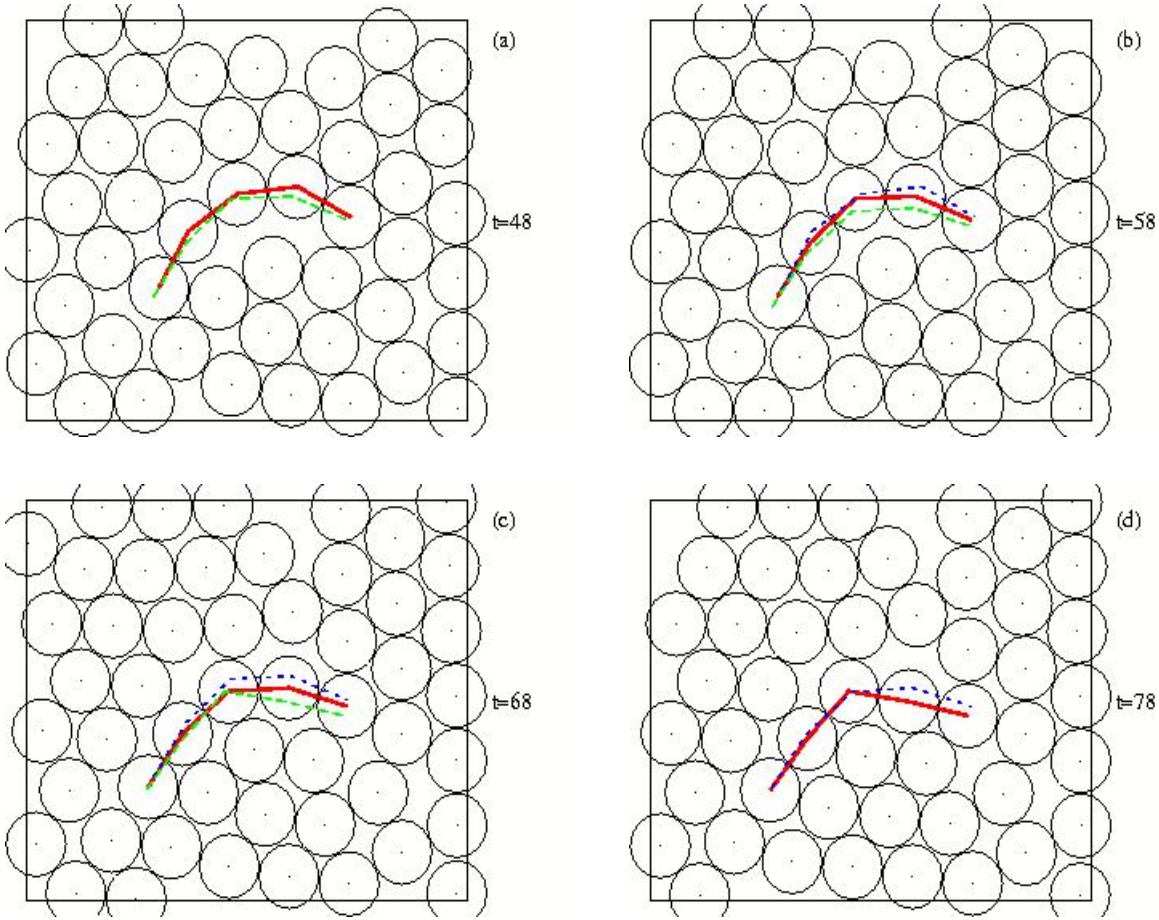
Granular materials (3)

- Time dependence of the connectivity numbers



Granular materials (4)

- Evolution of a bridge



SCIENTIFIC COMPUTING LABORATORY

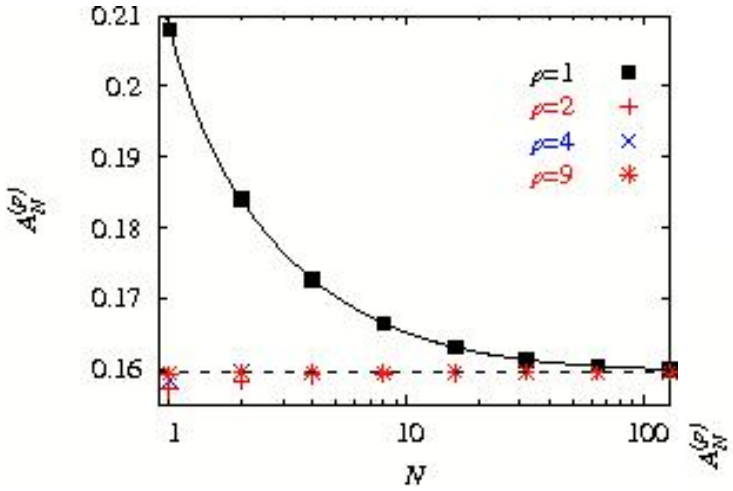
Path integrals (1)

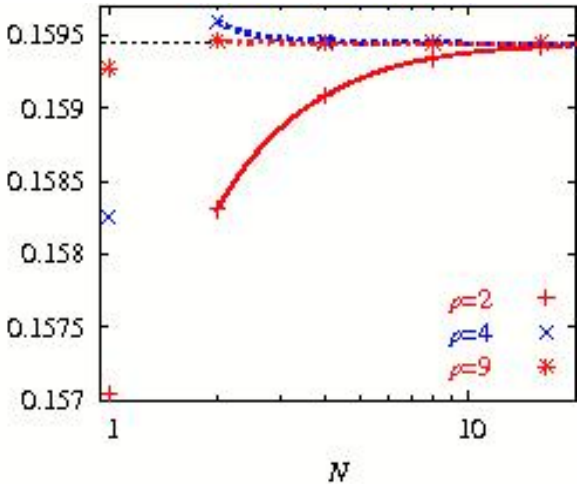
- Most economical way to write down a quantum theory
- Applications: physics, chemistry, materials
- Goal: devise $O(N^{-p})$ algorithm
- Previous state of the art: $O(N^{-4})$ for the trace and $O(N^{-2})$ for amplitude
- Tricks:
  use analytical information from generalized Euler summation formula
  invent a set of discreet effective actions $S^{(p)}$ with the same continuum limit
- Recent results:
  - A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. Lett.* **94**, 180403 (2005).
  - A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. B* **72**, 064302 (2005).
  - A. Bogojevic, A. Balaz, and A. Belic, *Phys. Lett. A* **344**, 84-90 (2005).
  - A. Bogojevic, A. Balaz, and A. Belic, *Phys. Lett. A* **345**, 258-264 (2005).
  - A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. E* **72**, 036128 (2005).
  - J. Grujic, A. Bogojevic, and A. Balaz, *Phys. Lett. A,* 217 (2006).
  - D. Stojiljkovic, A. Bogojevic, and A. Balaz, Phys. Lett. A 205-209 (2006).
  - A. Bogojevic, I. Vidanovic, A. Balaz and A. Belic, *Phys. Lett. A* **372** 3341-3349 (2008).
  - A. Balaz, A. Bogojevic, I. Vidanovic and A. Pelster, *Phys. Rev. E* **79** 036701 (2009)
  - I. Vidanovic, A. Bogojevic, A. Balaz and A. Belic, *Phys. Rev. E* **80** 066705 (2009).
  - I. Vidanovic, A. Bogojevic, A. Balaz and A. Belic, *Phys. Rev. E* **80** 066706 (2009).
  - A. Balaz, I. Vidanovic, A. Bogojevic and A. Pelster, *Phys. Lett. A* **374** 1539 (2010).
  - A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic and A. Pelster, *J. Stat. Mech.* P03004 (2011).
  - A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic and A. Pelster, *J. Stat. Mech.* P03005 (2011).
  - A. Balaz, I. Vidanovic, D. Stojiljkovic, D. Vudragovic, A. Bogojevic, A. Belic, *Comm. Comp. Phys.* in press (2011).

SCIENTIFIC COMPUTING LABORATORY

Path integrals (2)

- Descreete amplitudes for anharmonic oscilator





SCIENTIFIC COMPUTING LABORATORY

Path integrals (3)

- Deviations from the continuum limit