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New opportunities(?) for BOINC in the field of scientific simulation

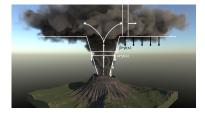
Bastien Chopard

Computer science Department, University of Geneva, Switzerland

CERN BOINC Workshop, May 29, 2024

Possible Application for home computing

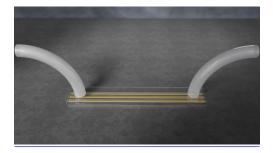
- Biomedical applications
- Volcanic ashes
- Emergence of life
- Computational Diplomacy



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1. Transport, Adhesion and Aggegation of Blood Platelets

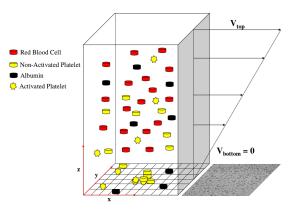
Platelets function analyzer



Could BOINC be used for the rendering of the frames of this movie?

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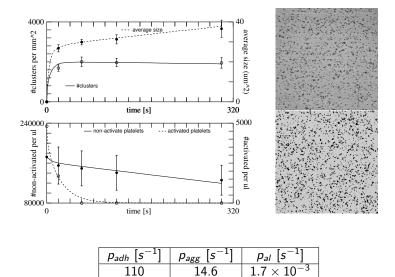
Mathematical "forward" model



Determine, from the deposition pattern, the platelets properties,

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Results (whole blood from 7 donors)



Determination of platelet properties

Use Machine Learning to determine these parameters Approximate Bayesian Computation

$$Prob(\theta|Obs) = \frac{Prob(Obs|\theta)Prob(\theta)}{Prob(Obs)}$$
$$\theta = (p_{Ag}, p_{Ad}, p_T, p_F, \ldots)$$

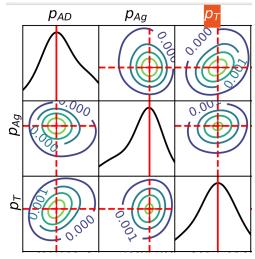
Determination of platelet properties

 $\mathrm{Prob}(\mathrm{Obs}|\theta)$ is obtained by sampling, \rightarrow distributed computing ABCpy software, using MPI

• R Dutta et al. Frontiers in Physiology, 'Advanced HPC-based Computational Modeling in Biomechanics and Systems Biology', Vol 9, article 1128. Front. Physiol. doi: 10.3389/fphys.2018.01128, 2018.

• R Dutta et al. PLoS Comput Biol 18(3): e1009910, 2020

Probability Distributions of platelets properties

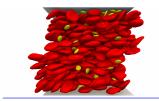


Based on 8 COPD patients

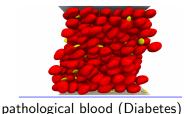
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Our mathematical model relies on some questionable hypotheseses

Need to determine the transport properties from fully resolved simulations (npFEM-Palabos)

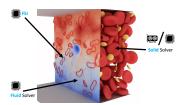


Healthy blood



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We need HPC capabilities (which excludes the home computing approach)



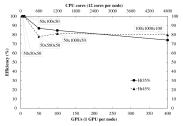


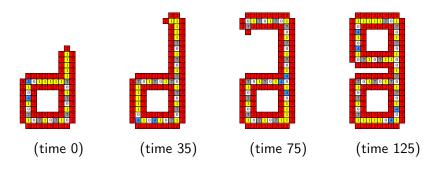
Figure 3.3 – Weak scaling efficiency for various domains at different hematocrit. To better understand the problem sizes consult table 3.1. The efficiency corresponds to the hybrid version of the code. The GPU nodes in Piz Daint are equipped with 12 cores and one NVIDIA GPU each.

About 5.5 days of supercomputer for 1 second of physical time.

2. Emergence of life: a possible application for citizen science?

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Can Cellular Automata generate artificial life forms from evolution?



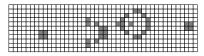
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Animation step by step

See C++/Langton/langton 200 200 600 601

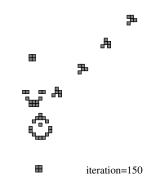
Emergence of Life: Conway's game of life

Emergence of complex structures in simple systems A glider gun



- A glider gun is a structure that keeps creating gliders
- There are more complex structures with more complex behavior: a zoology of organisms.
- The game of life is a Universal computer

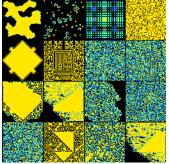
Animation step by step



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Emergence of life out of evolution.. or art generator

How long does it take to build a complex organism? How to simulate environment?



Combines CPU with human observations and analysis capabilities

Distributed optimization methods such multipopulation Genetic Algorithms are a way to have all machines collaborate.

(See also Tierra Artificial life: competition of programs)

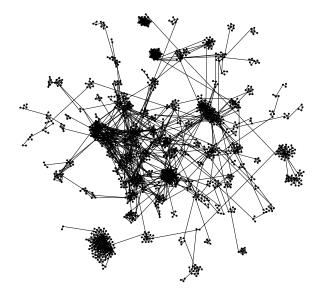
3. Computational Diplomacy



Bringing science into multilateral diplomacy Entablished in 2021 by ETH Zurich and UNDAT, the Science in Diplomacy Lab brings scientific insights and methods into diplomatic, international conflict resolution and help admit the global challenges our societies are facing.

- Create a new academic, open field
- Science in Diplomacy Laboratory: https://sidlab.ch
- Use modern methods of computational science to move the frontirers of science.
- Analyze international relations, multilateralism as a complex system
- The Diplodocus plateform

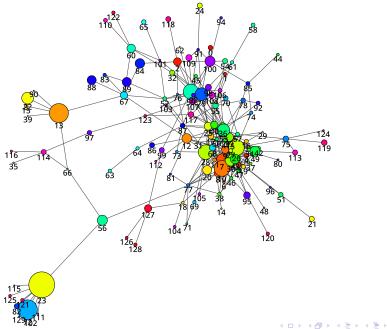
WHO resolutions: network of citations (1948–2021)



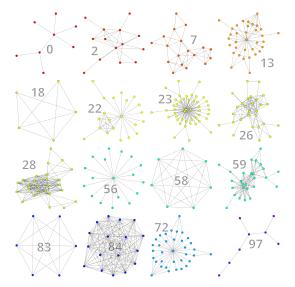
Credit: J.-L. Falcone, D. Wernli

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WHO resolutions: network of citations: communities



WHO resolutions: network of citations



- 0: governing
- 2: peace, disarmament
- 7: blindness, rehabilitation
- 13: invoking article
- 22: contributions,
- 23: assessment, members
- 26: drugs, antimicrobial resistance
- 28: infant
- 56: assessed contributions
- 58: international decade world, world indigenous people
- 59: developing countries
- 72: assessment future years
- 83: lesotho swaziland, struggle southern
- 84: displaced persons cyprus
- 97: coordination united nations

Most relevant words in resolution title

Computational Diplomacy

- Use a plateform as BOINC to combine human cabability to annotate documents (OCR) to help NPL algorithms.
- Help the scientists to build **Diplodocus**, a database for computational diplomacy that relies on texts written in natural languages.

3. Stresses the basic principle that the future of the Palestinian people cannot be discussed in their absence and, therefore, calls once more for the invitation of the Palestinic Liberation Organization, the representative of the Palestinic history of the Palestinic history

4. Endorses the recommendations of the Committee on the Exercise of the Inalienable Rights of the Palestinian. People contained in paragraphs 45 to 48 of its report and draws the attention of the Security Council to the need for urgent action thereon;

5. Reaffirms the inalienable right of the Palestinians to return to their homes and property in Palestine, from

Miled: Thirty-fifth Session, Supplement No. 35 (A/35/35). Thirty-fifth Session, Plenary Meetings, 75th meeting, paras. 83-141

ANNEX

Recommendations of the Committee on the Exercise of the Inalienable Rights of the Palestinian People, endorsed by the General Assembly at its thirty-first session⁴⁰

I. BASIC CONSIDERATIONS AND GUIDELINES

59. The question of Palestine is at the heart of the Middle East problem, and, consequently, the Committee stressed its belief that no solution in the Middle East can be envisaged which does not fully take into account the legitimate aspirations of the Palestinian people.

60. The legitimate and inalicrable rights of the Palestinian people to return to their homes and properly and to achieve self-determination, national independence and sovereignty are endorsed by the Committee in the conviction that the full implementation of these rights will contribute decisively to a comprehensive and final settlement of the Middle East craits.

⁴⁶The recommendations endorsed by the General Assembly in its resolution 31/20 were originally issued as part two of *Official Records* of the General Assembly, Thirty-first Session, Supplement No. 35 (A/31/35).

II. Resolutions adopted without reference to a Main Committee

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61. The participation of the Palestine Liberation Organization, the

III. RIGHT TO SELF-DETERMINATION, NATIONAL INDEPENDENCE

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THANK YOU FOR YOUR ATTENTION

Acknowledgments

H2020 center of excellence CompBioMed https://www.compbiomed.eu/



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- CSCS: grant for computing resources on Piz Daint
- Eureka-Eurostar project 3D-PLTs