The International Post-Exascale (InPEx) Project

SC23, Birds of a Feather
November 15, 2023 – rooms 301-303

Prof. Jack Dongarra, UTK

Prof. Pete Beckman, ANL

Dr. Jean-Yves Berthou, Inria

Prof. Satoshi Matsuoka, Riken R-CCS

Dr. Sergi Girona, BSC-CNS

Prof. Bernd Mohr, JSC

Dr. Emmanuel Jeannot, Inria

The International Post-Exascale (InPEx) Project

InPEx expected outcomes

- Formation of a solid network of exascale computing leaders, all around the globe
- Landmark documents largely exploited, worldwide, for supporting future post-exascale science
- Contribute to the implementation of an international, shared, high-quality computing environment based on the principles and practices of co-design

Actions:

- International Post-Exascale (InPEx) workshop series
- Dedicated international working groups

Participants:

Researchers, engineers (comp. science, math, application domains), HW&SW, industry, funding bodies

How to contribute? Send 2 pages white paper to: inpex@inpex.science

Feedback from the subgroups of the pre-meeting

- Meeting in Reims (France), October 19/20, 2023 : https://numpex.irisa.fr/international-collaborations-and-inpex-workshops/
- 6 subgroups :
  1. **Software production and management:** packaging, documentation, builds, results, catalogs, continuous integration, containerization, LLVM, parallel tools and sustainability. – Bernd Mohr (JCS), Bruno Raffin (Inria)
  2. **HPC/AI convergence:** ML, LLM for science, open models and datasets for AI training – Pete Beckman (NAISE), Jérôme Bobin (CEA)
  3. **Energy and environmental impact and sustainability** – Michèle Weiland (EPCC – University of Edinburgh), Georges Da Costa (IRIT)
  4. **Future and disruptive SW & HW technologies and usages (including accelerators)**: roadmaps, adoption... – Jack Dongarra (Univ. Tennessee), Jean-Yves Berthou (Inria)
  5. **Co-design, benchmarks/mini-Apps/Proxy and evaluation (HW & SW & Applications)** – Jean-Pierre Vilotte (CNRS), Masaaki Kondo (Riken CCS)
  6. **Digital Continuum and Data management** – Francesc Lordan (BSC), François Bodin (Univ. Rennes)

We neet to focus on the « HOW ». We want concrete outcome: science and technology (not only problems)

1. Software production and management

Context:

- Machines are getting more heterogeneous (CPUs, GPUs, mem. hierarchy, storage, network), and thus more difficult to program
- HPC software stack is getting more complex, build from an assembly of different components (HPC+HPDA+AI)
- HPC software is expected to interconnect with non-HPC components for building workflows in the Compute Continuum

Problematic(s):

- Development productivity
- Compilation and deployment
- Performance testing/portability
- Reproducibility
- Common software stack for HPC+HPDA+AI ??

1. Software production and management

Conclusions:

- Make it easier for exisiting users to share software products
- Can me make spack / module / easybuild / guix-hpc interoperate?
- Collaborate on container sharing (if software stack somewhat converge) and test within CI/CD pipelines
- Survey AI stacks and ensure we have a compatible software environment
- Increase productivity for users on our systems, situation is different than for AI as we have more variety

Main Actions:

- Survey on software tools/libs used in the different groups
- Create a mailing list (using emails of people in this working group room).
- Share working group spreadsheets (US/RIKEN working group list).
- Share with European colleagues and identify additional people to join collaboration, focus on action items above).
- Collaboration within the high performance software foundation (https://hpsfoundation.github.io/)?

2. AI for science / Science for AI

AI for science (HPC)

- As an “accelerator” (solvers, surrogate models, in-situ data analysis, code coupling etc.)
- A game-changer in applications (e.g. very fine-grain simulations, digital twins, inverse design, HPDA)
- AI-centric HW for HPC
- Dev. Productivity (e.g. LLM for code generation/conversion)
- Other impact ?

Science (HPC) for AI

- HPC data/compute workflows
- HPC tools for large model training/meta-learning (e.g. solvers, IO, task scheduling, etc)
- Energy/performance measurement/profiling
- Other impact ?

Problematics

1. **AI models for HPC**
    1. Common models for HPC applications ?
    2. Model validation/robustness/trust
    3. Flexible/extendable models
2. **How HPC can benefit from AI-centric dev ?**
    1. HW convergence, WS stack convergence ?
    2. Data everywhere in current/future systems/applications, can we benefit/reuse parts of the AI-centric tools ?
    3. Composability: e.g. interfacing with AI frameworks (e.g. pytorch, tensorflow, etc.)

2. AI for science / Science for AI

Action plan:

- The hard work is going from raw data to usable AI data and model
  - **Each InPeX community provides: Fully explained: open code, published data, from start to finish, presents their work at future workshops**
- **“The Pile” for Science**: large training data set available for foundation mode
  - Work together to share large, open scientific datasets for training and testing
  - **Each InPeX community ADDS their dataset to a unified, large set useful for building LLMs or multimode GPT**
- We must publish data in the form suitable for the AI community
  - We can identify and publish challenge problems
- Large foundation models for science
  - TPC (https://tpc.dev)
  - Many groups are working on building their own small models, specialized for their community
  - FugakuGPT and AuroraGPT. The EU strategy on AI4Science must be clarified
- Can we make strong statements about ***Scientific AI*** (reproducibility, trustworthy, explainable)?
  - **Development of shared concepts and language for discussing and comparing**
- Coordinated, shared path to connect with broader AI community
  - Clear explanation that international AI infrastructure is available in national investments
  - Better organize linking of AI and Science communities
  - HuggingFace, Allen Inst, etc.

3. Energy and environmental impact and sustainability

Context:

- Several levels: Hardware (including datacentre); SW Stack; Applications.
- Available leverages:
  - Conventional: Improve hardware, software, compilers, numerical libraries, scheduling, dynamism (tasks-based applications)
  - Unconventional: reconfiguration of applications, of hardware; power capping, approximate computing; cross-system scheduling
- New constraints: curtailment; CO^2 and energy reporting and budget.

Problematics:

- Power and Energy reduction
- CO^2 impact
- Cost for users
  - At the cost of performance?
  - At the cost of usability / portability / code sustainability?
- Education: even fundamental understanding is lacking

3. Energy and environmental impact and sustainability

Conclusion:

- Priority is science, and the goal is to optimize CO^2 per « *Nobel Prize* »

Actions:

- [Lobbying] Clarify the political expectation and their societal impact
- [Tool] Providing feedback to users: Eq. CO^2, Wh, up to abnormal behavior for certain libraries
- [Workshop] Discussion on metrics: how to improve Green500, etc.
- [Workshop] Session on success stories and actual failures of pre-exascale operators
- [Workshop] Challenge for students/researchers: use actual application on a datacenter to reduce power consumption while keeping the same/acceptable performance
- [Workshop] Processor technologies - e.g. reducing standby power consumption
- [MOOC] User education

4. Future and disruptive SW & HW technologies and usages

Problematics

- What technologies **available today** are disruptive?
- What **future** disruptive technologies ?
- **Other impact** of disruption?
- For what **uses, for what impact?**

Opportunities/game changer and threats

- IA and HPC (IA-code generator, IA-solver, …)
- Disruptive Hardware Technologies (Chiplet, Neuromorphic Computing, Optical Computing, DNA Storage and Computing, Graphene-Based Processors, Silicon Photonics , Quantum Computing)
- Disruptive Software Technologies (Containers, Quantum Computing Software ?)
- Disruptive trends for data management (Emerging storage technologies, disaggregated memory (CXL), compute (FPGA) and storage resources, Leverage fine-grain I/O monitoring information, energy limit for the power consumption, Risk: some storage technologies could be stopped (e.g., Intel Optane))

4. Future and disruptive SW & HW technologies and usages

Action Plan

Action 1, InPEx workshops, applications + AI:

- Invite different communities to exchange on opportunities and results obtained using IA
- Use ambassadors who are already convinced to spread the message

Action 2 (longer term): organize domain scientific challenges (climate, astro, bio, ….) where AI might be a game changer

Action 3: Quantum computing: share access to our infrastructures in EU/Japan/US, testing different implementations of quantum facilities, experimenting different programming models, mathematical libraries, training, …

Action 4. Identifying game changer among possible disruptions (disruptions that change practices and impact)

> **Action 4.1** InpEx workshop, organize a session dedicated to
>
> - Chiplets
> - DNA storing is coming (may replace tape rapidly)
> - Photonics
> - Quantum algorithms (coupled infra)
> - Disagregation memory
> - Goal: identify opportunities it opens, new practices, impact
>
> **Action 4.2** Funding, support exploratory projects with funding

5. Co-design, benchmarks/mini-Apps/Proxy and evaluation

Context:

- Exascale Computing Project (ECP)
- Fugaku & Fugaku NEXT co-design projects
- Euro-HPC JU initiatives
- ETP4HPC

Problematics:

- Comp. sc. eng. applications development methodologies, accuracy & performance portability
- Co-designed software-Stack/Applications
- Proxy-apps / mini-apps suites
- HW & SW Integration, Testing & Profiling tools, Benchmarking specifications

5. Co-design, benchmarks/mini-Apps/Proxy and evaluation

Actions

3 identified sessions (software stack developers, application developers) for the next InPEx workshop

1. Efficient application developpment at exascale and beyond
   - leveraging existing tools (e.g., MFEM, Lib-Paranuma, Lib-CEED, MAGMA, PetSc, OCCA-API, Kokkos, Raja, …)
   - address gaps and missing functionalities
2. Develop, coordinate and shared application-driven proxy-apps and mini-apps suites
   - identify and share proxy-apps and mini-apps with standardised specifications, performance analysis methodologies, metrics and shared results
   - build shared distributed information system (repositories, GitHub, gitlab ....)
3. Performance portable programming models and abstraction level:
   - International coordination, collaboration in the development of core components in a co-design way
   - Increase awareness and use of performance programming models in CSE applications development

6. Digital Continuum and Data management

Context:

- Edge low-adoption technology but there is interest
- Cyber-physical systems are being used for data collection
- Digital Continuum is currently being driven by large Cloud Providers

Problematics

- HPC centers compete with Cloud Providers
  - What has HPC to offer compared to Cloud Providers?
- Real-time data with real-time processing requirements
- Digital Continuum is a multi-tenant environment.
  - Collected data used with multiple purposes
  - Computing Infrastructure is also shared

6. Digital Continuum and Data management

Actions:

- Build a continuum of trusted entities:
  - How to trust data exchanges in the continuum?
    - How to ensure sensor data veracity (proof of provenance)
    - How to ensure connections source / destination
  - How to cloudify HPC/IA services?
- Building a continuum related PoC using multiple infrastructures
  - Find a good candidate application
- Participation of the "architecture" EU definition of the continuum
  - https://eucloudedgeiot.eu/task-forces/architecture-tf3/

The International Post-Exascale (InPEx) workshop series

Organization, agenda and funding of Inpex workshops

- Host country covers all accommodation and food costs, each participant cover their own travel costs.
- Two or three days, keynotes and breakout sessions on specific subjects
- Participants : researchers, engineers (comp. science, math, application domains), HW&SW, industry, funding bodies
- Reducing CO^2 impact: enabling remote participation

Date	(10/2023)	11/2023	06/2024	06/2025
Location	Preparatory phase EU (France)	SC’23 - BOF	Workshop1 EU	Workshop2 Japan
Date	03/2026	09/2026	06/2027	09/2027
Location	Workshop3 US	Workshop4 EU	Workshop5 Japan	Workshop6 US

Pre-workshop InPEx, October 2023, Reims, Fr
https://numpex.irisa.fr/international-collaborations-and-inpex-workshops/

How to contribute? Send 2 pages white paper to : inpex@inpex.science