(SICM)$^2$ Parallel Computing Workshop

Attendees

Chemistry
Daniel Crawford  PSI, many-body
Sarom Leang  GAMESS
Edoardo Apra  DFT, NWChem
Eduard Valeev  Many-body, MPQC
Ilya Kaliman  Many-body, QChem
Gary Trucks  Gaussian
Bryan Sundahl  TDFT, NWChem, MADNESS
Lubos Mitas  QMC
Robert Harrison  NWChem, MADNESS

Materials
Robert DiStasio  Plane wave DFT, Quantum Espresso, QChem
Jack Deslippe  Real space DFT, PARSEC
Scott Thornton  DFT and GW, misc
Paul Crozier  Molecular dynamics, LAMMPS
Markus Eisenbech  Many-body, DCA++

Computer science
Beverley Sanders  SIAL, ACES
Laximant Kale  Molecular dynamics, Charm++, NAMD
Bradford Chamberlain  Languages, Chapel
Sriram Krishnamoorthy  Global Arrays, NWChem
Anthony Danalis  DAG-based methods
P. Sadayappan  Tensors, polyhedral optimizer
Yonghong Yan  OpenMP
Draft Agenda

Friday 6-9pm SUNYRF Global

6:00-6:05 Welcome

6:05-6:30 Crawford – S2I2M2 vision and status

6:30-9:00pm Chemistry and Materials – challenges and opportunities

6:30-7:00 Harrison – Workshop objectives, challenges and opportunities

Subsequent presentations to address these questions

- Summary of the science domain
  - Example applications(s) in 2020
  - What drives the frontier? Size, time, sampling, ...
  - How big are the user and developer communities?
  - What types and scale of computing are relevant in 2020
    - Lots of terascale jobs? Petascale? Exascale?
  - Computational algorithms
    - E.g., Mesh, FFT, linear algebra, ...
    - Relevant dimensions, memory capacity, floating point intensity, ...
    - How will these change by 2020?
  - What languages, parallel programming models, etc., are used in this domain?
  - What are your current plans for 2020?
  - With regard to sustaining HPC software in your domain
    - What up to 3 success stories exist now?
    - What are the top 3 challenges now?
    - What do you see as the top 3 challenges in 2020?

7:00-9:00 Chemistry materials talks – each talk is 15 minutes

- Trucks – View from Gaussian/industry
- Apra – Gaussian molecular electronic structure
- Mitas – QMC
- DiStasio – Plane wave DFT
- Deslippe – Real space DFT
- Crozier – Molecular dynamics
- Eisenbach – Many body
- Wrap up and plans for next day
Saturday SUNY Manhattan

9:00:11:40am  Computer science – challenges and opportunities

Subsequent presentations to address these questions
•  What is your elevator story for the scientists?
  ◦  A little detail behind the elevator story
  ◦  Present and future challenges in HPC
  ◦  Your vision/approach to parallel programming
•  With regard to designing and programming HPC codes
  ◦  What up to 3 success stories exist now?
  ◦  What are the top 3 challenges now?
  ◦  What do you see as the top 3 challenges in 2020?
•  How should scientists be thinking of a sustainable path forward?
  ◦  How can we drive relevant standards?
  ◦  How can we help enable relevant innovations?
  ◦  What must/can/should we do for ourselves?
•  Roles for computer science research, students, and products in the institute?

Each of the following is 20 minutes
•  Laximant Kale – Charm++, NAMD
•  Beverley Sanders – SIAL, ACES
•  Sriram Krishnamoorthy – Global Arrays, Resilience
•  Anthony Danalis – DAG-based composition
•  Break
•  P. Sadayappan – Tensors, polyhedral optimizer
•  Yonghong Yan – OpenMP
•  Bradford Chamberlain – Chapel, life, the universe

11:40-11:50  Quick break

11:50-12:45  Discussion as big group
  Objective: Mind meld on objectives and initial path forward for the break out sessions

12:45-1:45  Lunch (box lunch provided)
1:45-3:15  
*Breakout session 1 (90 minutes)*
Attendees will be pre-assigned to sections

*Breakout A. Molecules*

*Breakout B. Materials*

Objectives:
- Identify challenges and opportunities
- What do we need to expand participation?
- What do we need to accelerate discovery/innovation?
- Current state of art in science domain
- Science drivers for 2020
- Characteristics of computation in 2020
- Opportunities and road blocks
- Who/what is not in the room?
- What should a sustainable approach aspire to?

3:15-3:30  
*Break*

3:30-5:00  
*Breakout session 2 (90 minutes)*
Attendees will be pre-assigned to sections

*Breakout C. Emphasizing productivity*

*Breakout D. Emphasizing performance*

Objectives:
- Identify challenges and opportunities
- What do we need to expand participation?
- What do we need to accelerate discovery/innovation?
- What are absolute must dos?
- What are conservative reliable approaches?
- What are blue sky potentially transformational approaches?
- Who/what is not in the room?
- What should a sustainable approach aspire to?

5:00-5:15  
*Break*

5:15-6:00  
*Big group (45 minutes)*
- Summary presentations and discussion
- Discuss agenda and objectives for Sunday
Sunday SUNY Manhattan

9:00-10:30  Breakout session 3 (90 minutes)
Attendees will be pre-assigned to sections

Breakout E. Education

Breakout F. Community, collaboration, architecture

Objectives:
• What should we be teaching?
• How should we organize?
• How do we maintain our brands and yet develop communally?
• Two-way educational efforts: Can we train domain scientists in just enough software design and computer scientists in just enough science to make serious progress?
• Giving credit for thankless work: how can we ensure that those developing infrastructure are recognized for their efforts?
• Career opportunities: Can developing tools rather than methods yield desirable permanent positions?
• What kind of environment, people, and resources provide the best opportunity for serious collaboration between computational scientists and computer scientists? Can any sort of top-down effort succeed?
• How broadly should our community be defined? Are our software challenges for large-scale computing sufficiently similar that we're part of the same tribe?

10:30-10:45  Break

10:45-11:45  Big-group discussion

11:45-2:00  Working lunch (box lunch provided)