The Co-Design Process for Scientists and Project Leads

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Should I be interested in GPU-enabling my science?

What do we mean by co-design?

- Designing projects based on hardware characteristics, software constraints, and science objectives.
- What science could GPU-enablement really advance?
  - Some science objectives are well suited or GPU friendly
  - Other science objectives are not particularly GPU friendly
- This is not “Let’s do GPU-programming because everybody else is doing it”

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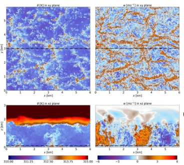
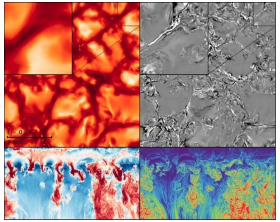
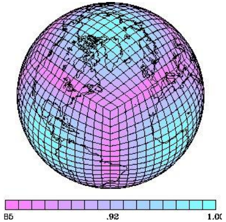
back-of-the-envelope calculation ahead

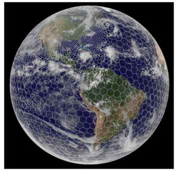
Multiple successful earth system applications that have been GPU-enabled

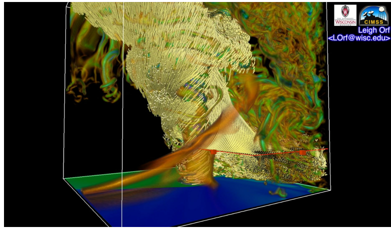


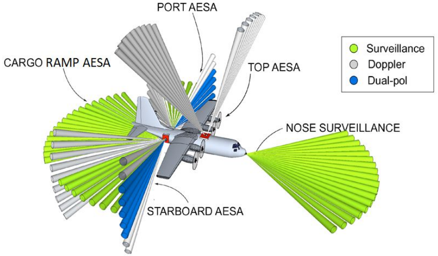




- FastEddy
  - Large eddy simulation (LES) code for microscale flows
- MURaM
  - Multidimensional MHD to study solar magneto-convection and other related magnetic activities
- CM1
  - Mesoscale atmospheric model used for idealized process studies
- MPAS-A
  - Atmospheric component of the Model for Prediction Across Scales
- SAMURAI
  - variational data assimilation of APAR observations
- HOMME++
  - Spectral element dynamical core used by the E3SM project







Common features of these GPU projects

- Compatible scientific objective
  - Have identified when a science objective is a good fit for GPU-enablement
- Knowledgeable, interdisciplinary team
  - Project design for GPU-enablement
  - Knowledge about how to perform the transformation
    - How to program in OpenACC, OpenMP offload, or CUDA
- Clearly defined achievable goals
- Significant stakeholder engagement
- Significant software engineering investments

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See other workshop sessions

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Outline

- Motivation
- How to identify GPU friendly science objectives
- Estimating effort to achieve GPU-enablement
- Estimating return on investment (ROI)

A collection of scientific objectives

- Unlikely to be GPU friendly
  - Paleo-climate
  - Climate change
- Likely to be GPU friendly
  - Climate variability using large-ensembles
  - Ocean modeling process studies
  - High-resolution whole atmosphere modeling with Data Assimilation
  - Reanalysis
  - Compute-intensive post-processing
  - Data assimilation of observational data
- Very GPU friendly
  - Numerical weather prediction
  - Seasonal to sub-seasonal forecasting
  - Regional ocean modeling
  - LES modeling
  - High-resolution regional modeling with complex chemistry
  - Space-weather prediction
  - magnetosphere modeling

How to determine if your science is GPU friendly

- Is it a computational demanding and why?
  - Potential scientific simulations
    - MPAS-A 3.75 km weather modeling
      - 38.6M x 56 ⇒ O(2162M) independent grid-points
      - ~300 GPUs per run: grid-points per GPU = O(7.2M)
      - O(1.22M) timesteps
    - CM1 ASD simulations
      - 2048x2048x1024 ⇒ O(4294M) independent grid-points
      - ~128 GPUs per run: grid-points per GPU = O(33M)
      - O(87K) timesteps
    - MURaM ASD simulations
      - 2352x2016x2016 ⇒ O(9559M) independent grid-points
      - ~252 GPUs per run: grid-points per GPU = O(37.9M)
      - O(250K) timesteps

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      -
  - Computational demanding because of <u>number of independent grid-points</u>!

GPU friendly configurations

How to determine if your science is GPU friendly

- Is it a computational demanding and why?
  - Other potential configurations
    - 1-degree climate change:
      - 288x192x32 ⇒ O(1.7M) independent grid-points
      - 64 nodes per run: grid-points per node = O(27K)
      - ~O(17M) timesteps
  - Computationally demanding because of <u>number of timesteps</u>!

Less GPU friendly

- Does it perform a large amount of calculations between I/O?
  - Example

```
read() Temp
avgTemp = SUM(Temp(:,:,:));
```

  - Efficient use of GPU minimizes off device transfers
  - I/O bound problems are not typically a good match for GPUs

How to determine if your science is GPU friendly (con't)

- Does the science have rate or throughput limitations?
  - If rate limitations
    - Execution rate GPU should match or exceed CPU rate ⇒ GPU friendly
    - Example:
      - Operational weather forecasting
      - Long climate simulations
  - If throughput limitations
    - Can more science be performed quicker or using less hardware
    - Example:
      - Large Eddy Simulation (LES)
      - large-ensemble climate modeling
      - seasonal to sub-seasonal forecasting
      - Magnetohydrodynamics (MHD)

Are your science objectives GPU friendly? [Student exercise: 13 minutes]

- Student exercise [5 minutes]

  - Determine the following
    - Total number of independent grid-points
    - # {nodes,GPU} per run
    - # grid-points per {node,GPU}
    - # timesteps per run
  - Does it perform I/O frequently?
  - Do you have rate or throughput limitations?

- Discuss as a group any interesting realizations [7 minutes]

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Estimating effort for GPU-enablement

- Does a GPU-enabled version of your code already exist?
  - Does this version of the code support all the necessary physics options?
- Is the code written in such a way that it is GPU-ready?
  - Is significant or full parallelism available at loop level?
  - Does a threaded (e.g. OpenMP) version of the code exist?
  - Does the code have some form of verification?

GPU-ready:
Is significant parallelism available at the loop level?

- Needing to rewrite call structure to support significant parallelism at the loop level can be very time consuming.
- Example: GPU ready loop arrangement

```
do k=1,1024
    do j=1,128
        do i=1,256
            wten(i,j,k)=wten(i,j,k)+(c1(i,j,k)*dum8(i,j,k-1)+c2(i,j,k)*dum8(i,j,k))
        enddo
    enddo
enddo
```

- Example: Loops in need of rearrangement

```
do k=1, 1024
    call radiation_solver()
    do j=1,128
        call lw_solve(a(1:256))
    enddo
enddo
```

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                enddo
        enddo
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Full parallelism available at loop level

- Example: Loops in need of rearrangement

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```

Limited parallelism at loop level

GPU-ready:
Does a threaded version of the code already exist?

- OpenACC and OpenMP offload constructs are very similar to existing CPU-based threading
- Existing threaded version indicates that parallel "issues" have already been considered
- Existing threading approach may need to be reworked
  - GPUs needs much larger level of concurrency

GPU-ready:
Does the code provide verification?

- Code verification allows for incremental GPU-enablement
- Much easier to retain correctness than to regain correctness
- Addressing correctness bugs typically take majority of code conversion time
- Presence of well designed code verification simplifies the time spent debugging GPU-enabled code

Is your code GPU ready? [Student exercise: 13 minutes]

- Student exercise [5 minutes]
  - Does a GPU version of your code already exist?
    - Yes [0 points]
      - Are the desired physics packaged GPU-enabled?
        - » Yes [1 points]
        - » No [3 points]
    - No [4 points]
  - Is the code writing in such a way that it is GPU-ready?
    - Is full parallelism is available at loop level?
      - Yes [1 points]
      - No [7 points]
    - Does a threaded version of the code exist?
      - Yes [1 point]
      - No [7 points]
    - Does the code have some form of verification?
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CM1

4

1

1

7

13 points

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Estimating Return on Investment (ROI)

- What kind of capability GPU-enablement will deliver versus existing CPU code?
  - Serial versus parallel base case?
- Potential advantages to creation of a CPU and GPU enabled code
  - Reduced time-to-discovery for a particular science question
  - Access to broader collection of hardware
  - Ability to perform more science for a fixed resource cost
  - Ability to perform science not otherwise possible
- Advantage of GPU computing a result of better memory bandwidth and Floating-point (FP) rates
  - For Derecho: NVIDIA A100 versus AMD EPYC 7763
    - 3.8x increase in memory bandwidth
    - 1.9x increase in theoretical FP32 & FP64 rates

What is the working set size for a tightly nested loop?

- Consider typical loop in CM1:

```
do k=1,1024
    do j=1,128
        do i=1,256
            wten(i,j,k)=wten(i,j,k)+(c1(i,j,k)*dum8(i,j,k-1)+c2(i,j,k)*dum8(i,j,k))
        enddo
    enddo
enddo
```

- Loop accesses: 4 variables, 4-byte reals, of dimension 128x256x1024
- Total data access 512 MBytes which exceeds the 256 MB L3 cache on AMD EYPC
  - Memory bandwidth limited calculation → 3.8x potential speedup
- Measured overall CM1 speedup: 3.9x

What is the estimated ROI? [Student exercise: 13 minutes]

- Student exercise [5 minutes]
  - What is your working set size for inner loops?
  - What kind of Return on Investment (ROI) would you expect?
  - Would this kind of ROI have a meaningful impact on your science?
- Discuss with group any interesting realizations [7 minutes]

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Additional resources:

- Co-Design in the Exascale Computing Project (paper), Tim Germann 2021
- ECP Co-Design Centers
- HPC Co-Design (conference briefing by NNSA to DoD), Ronald Brightwell 2017
- Workshop on Software Co-Design Actions in European Flagship HPC Codes, 2022
- Resources for Co-Design from POP Organization
  - Webinar recording by POP on this platform plus slides
- A Blueprint for Success: Co-Design Approach for the Modular Supercomputing Architecture (MSA), Intel 2020
- Truly Heterogeneous HPC: Co-Design to Achieve What Science Needs from HPC (slides), Smokey Mountain CSEC 2020 (focuses on neuromorphic computing)
- On the Role of Co-Design in HPC (paper), Barrett, et al 2013