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NCHC Open Hackathon 2024

Final presentation

GPU-Based Acceleration VVM Team

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LCDM
Lab. for Cloud Dynamics and Modeling

ATMOSPHERIC ENVIRONMENT LAB

special thanks to 尚恩

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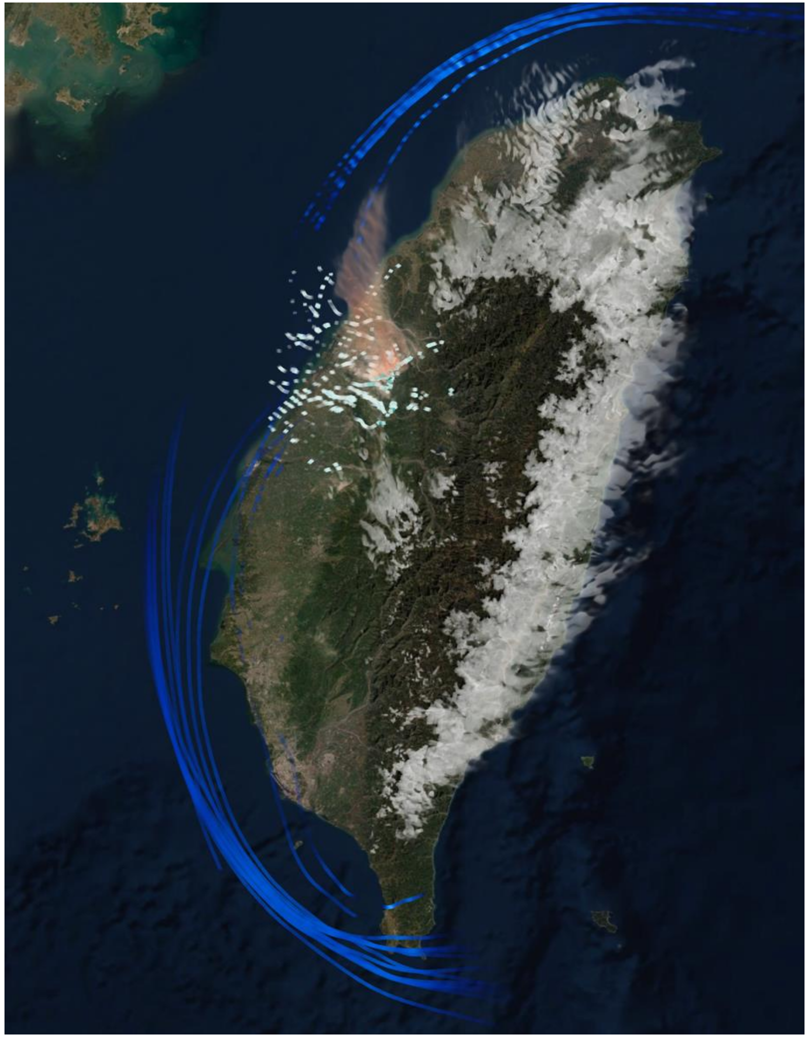

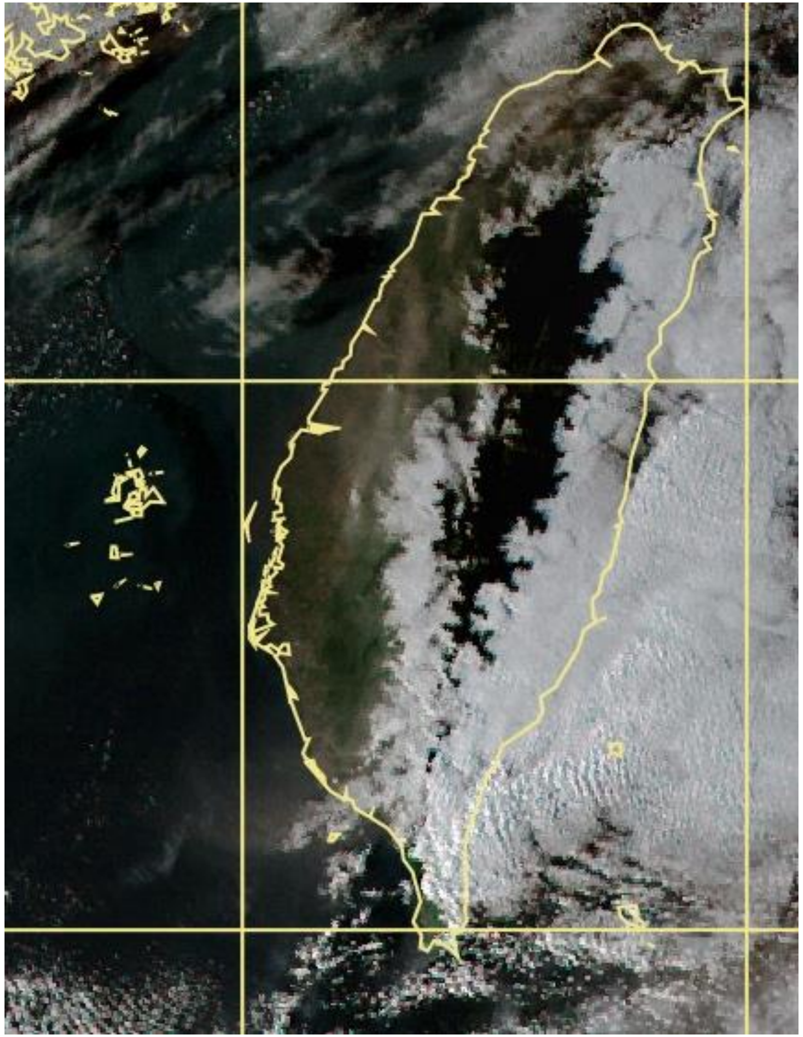

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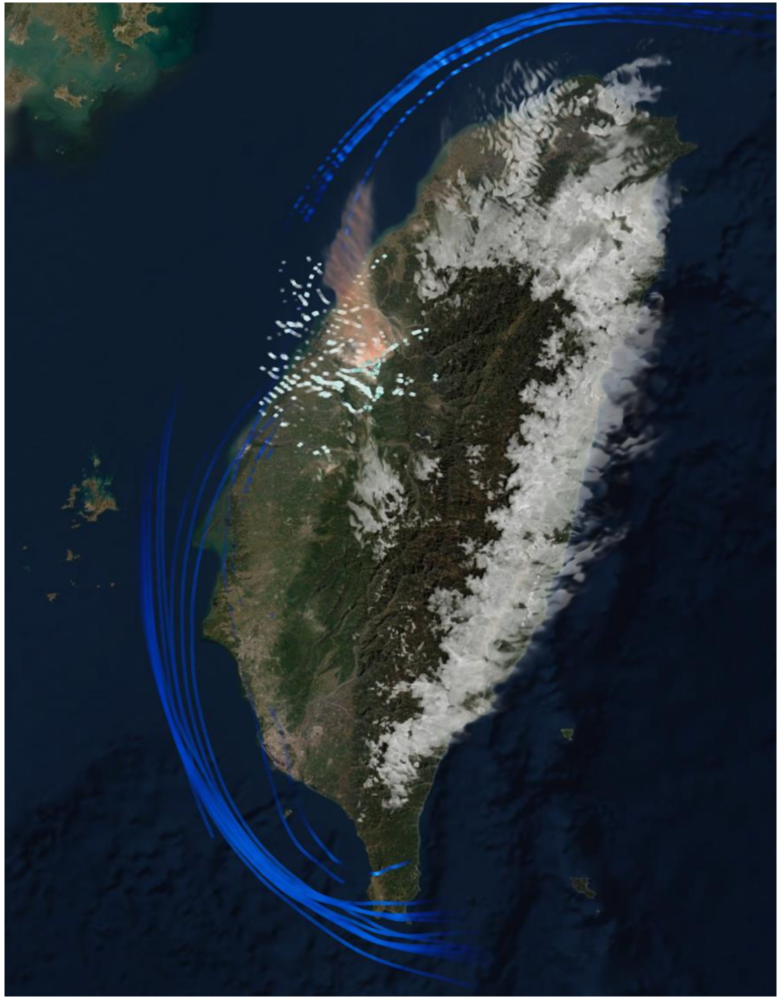
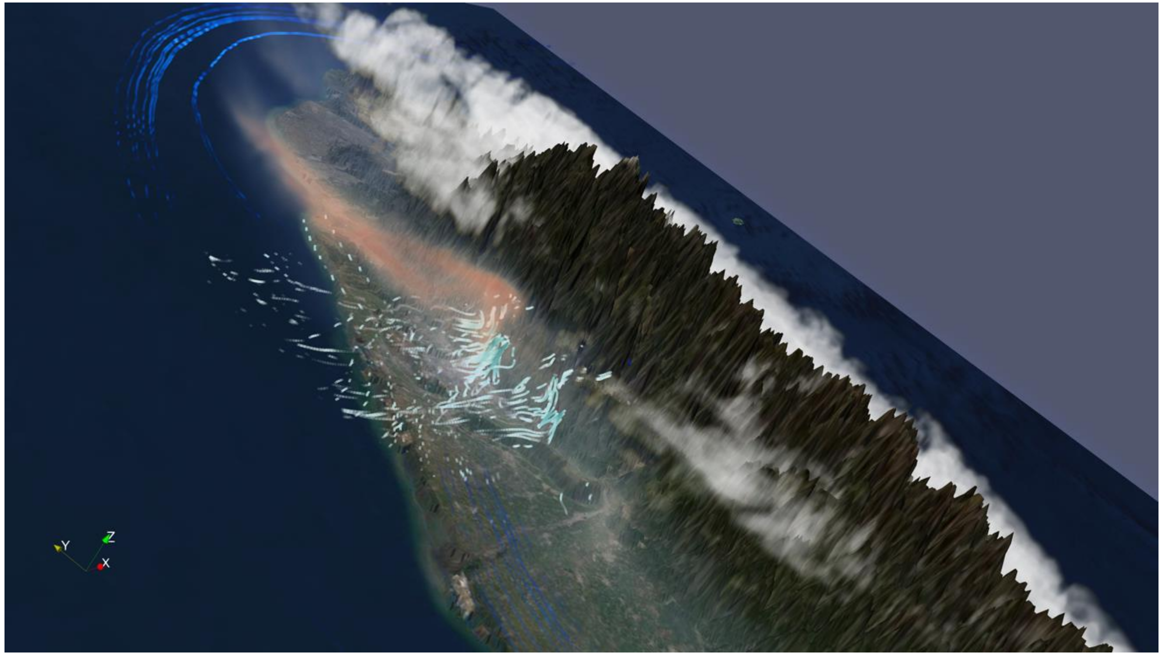
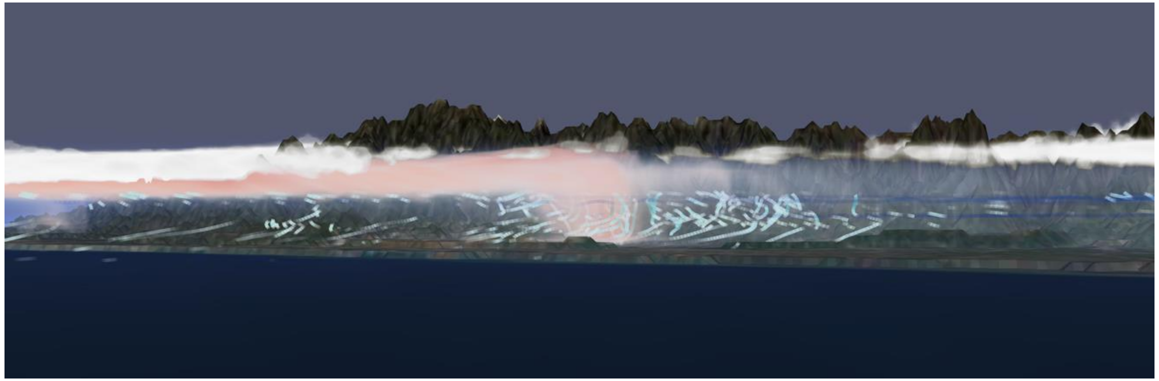
Clouds, Rain, and Pollution





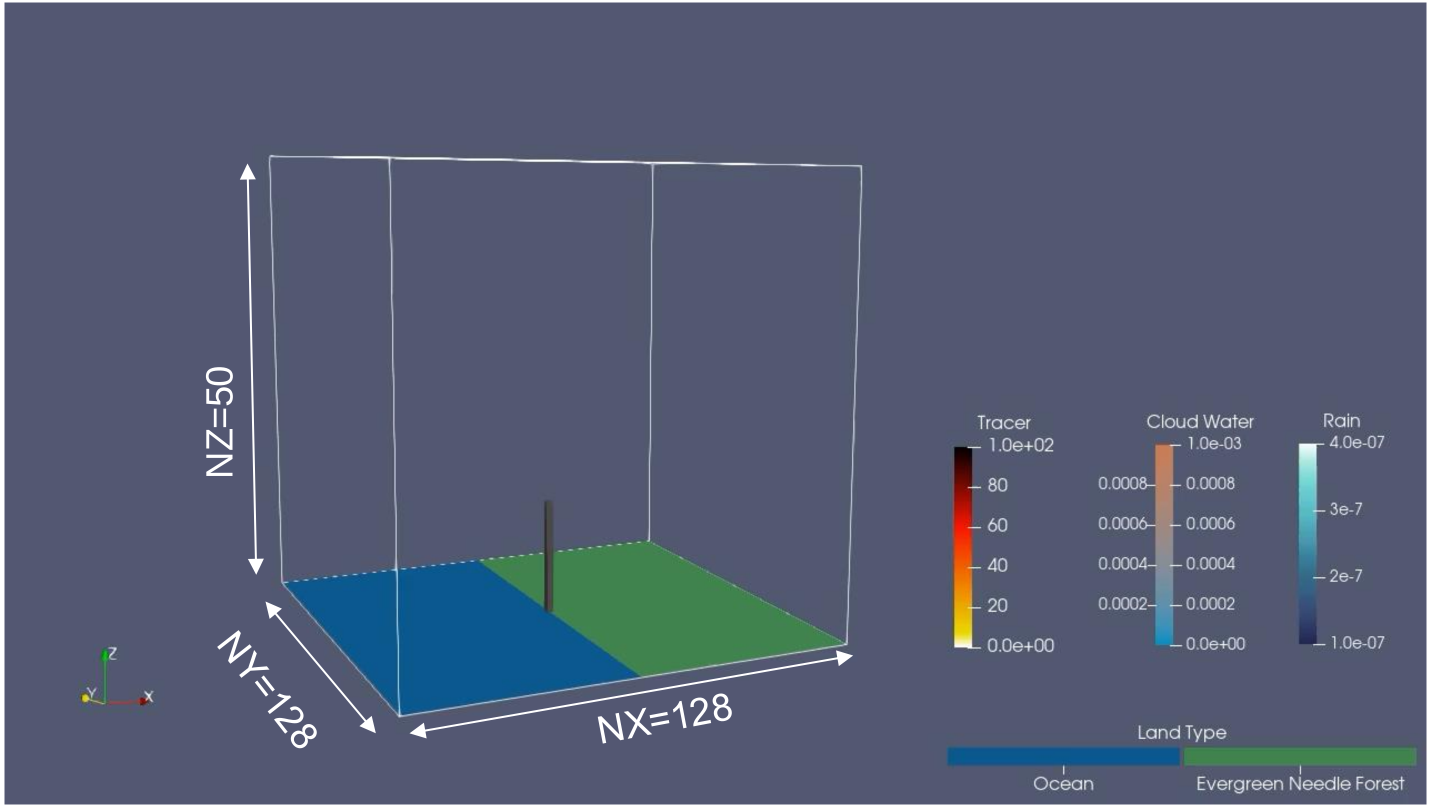


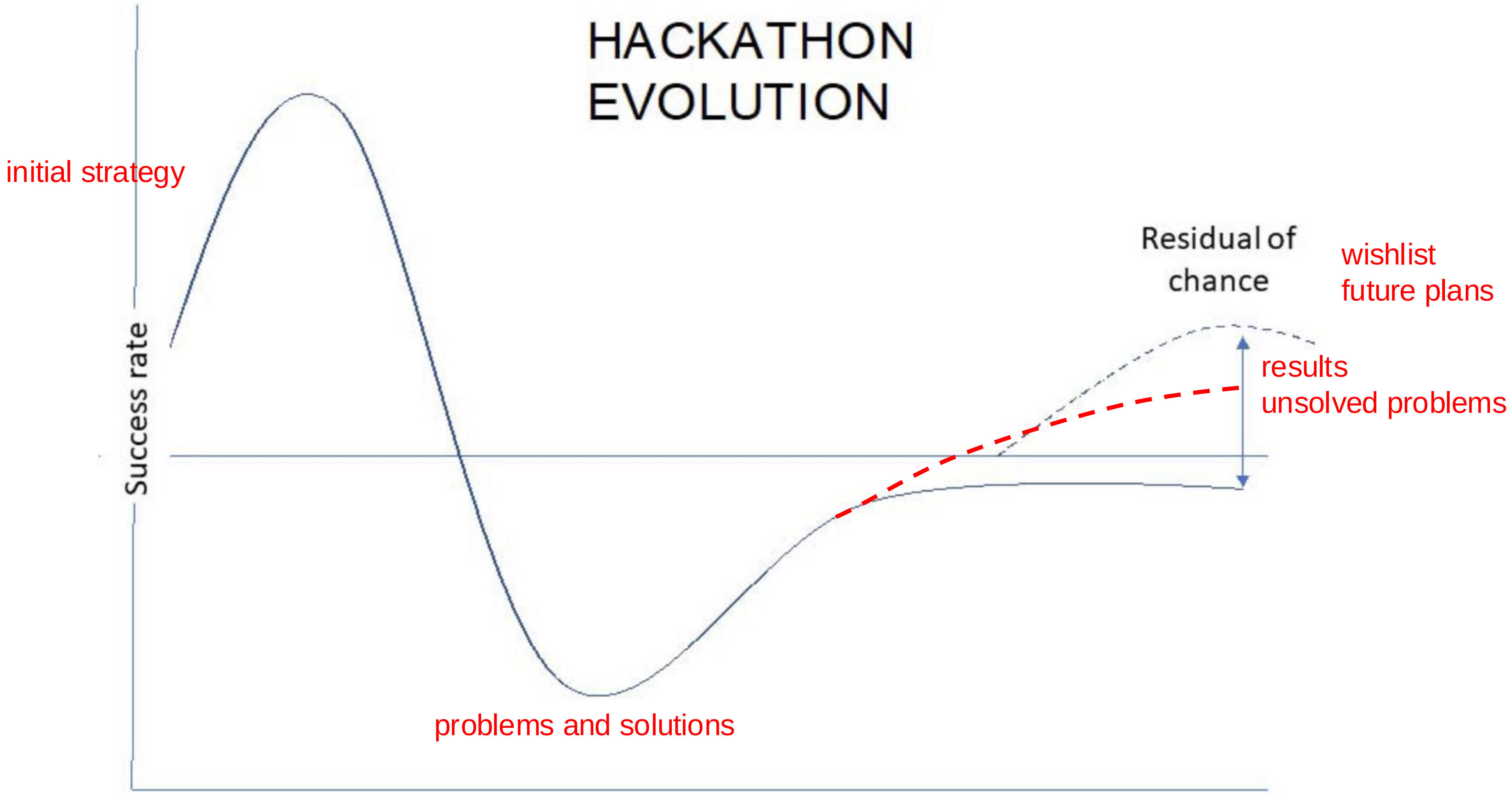
*14000 CPU hour for a 24-hr simulation

Atmospheric Physical and Chemical Processes Simulation using Vector Vorticity equation cloud-resolving Model (VVM)

- Fortran code
- 4-core CPU with MPI
- Domain: 128x128x50
- integrates 720 steps

  (2 hours)

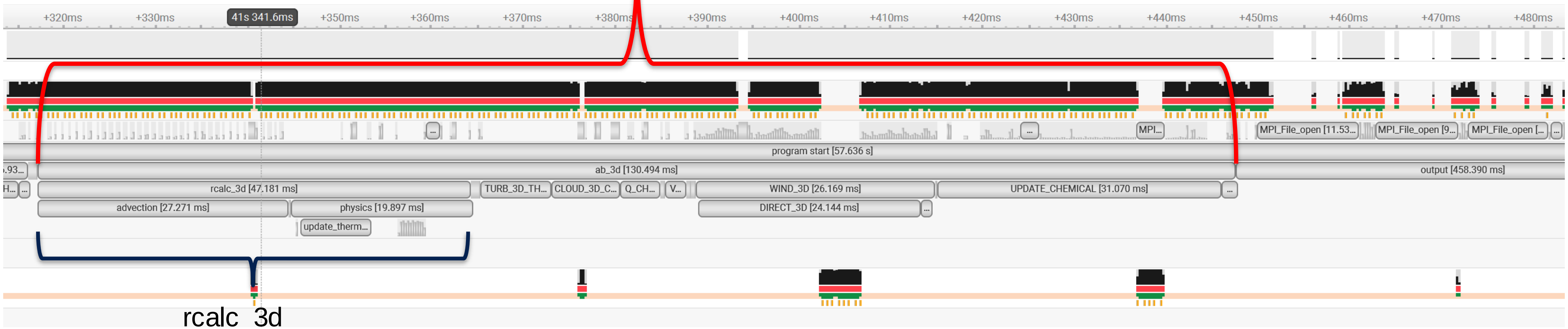




Chandrasekaran et al., (2018)
doi: 10.1109/MCSE.2018.042781332.

initial strategy

ab_3d (one step), 130.5ms



rcalc_3d

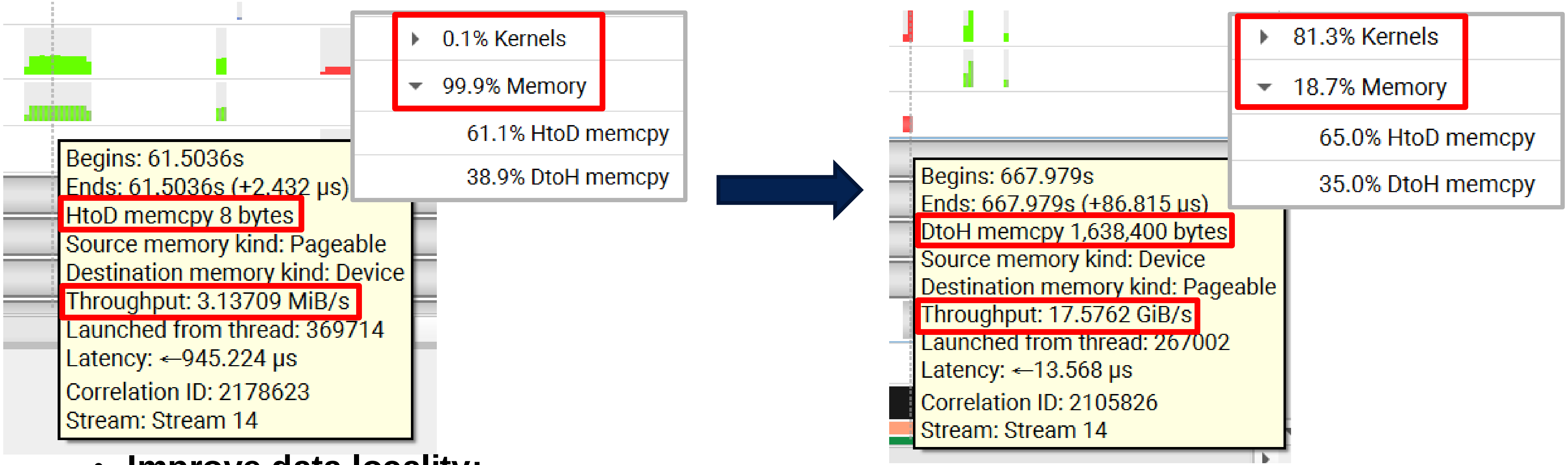
advection
20%

wind_3d
(direct_3d 18%)

UPDATE_CHEMICAL
23%

- porting path: openACC multi-core → openACC GPU

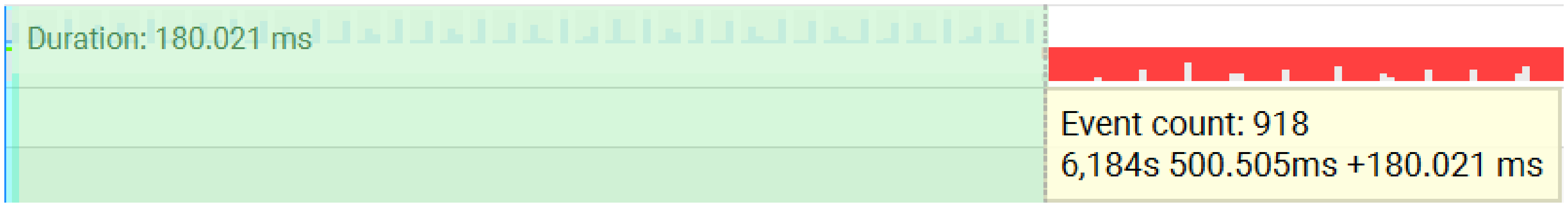
problems and solutions

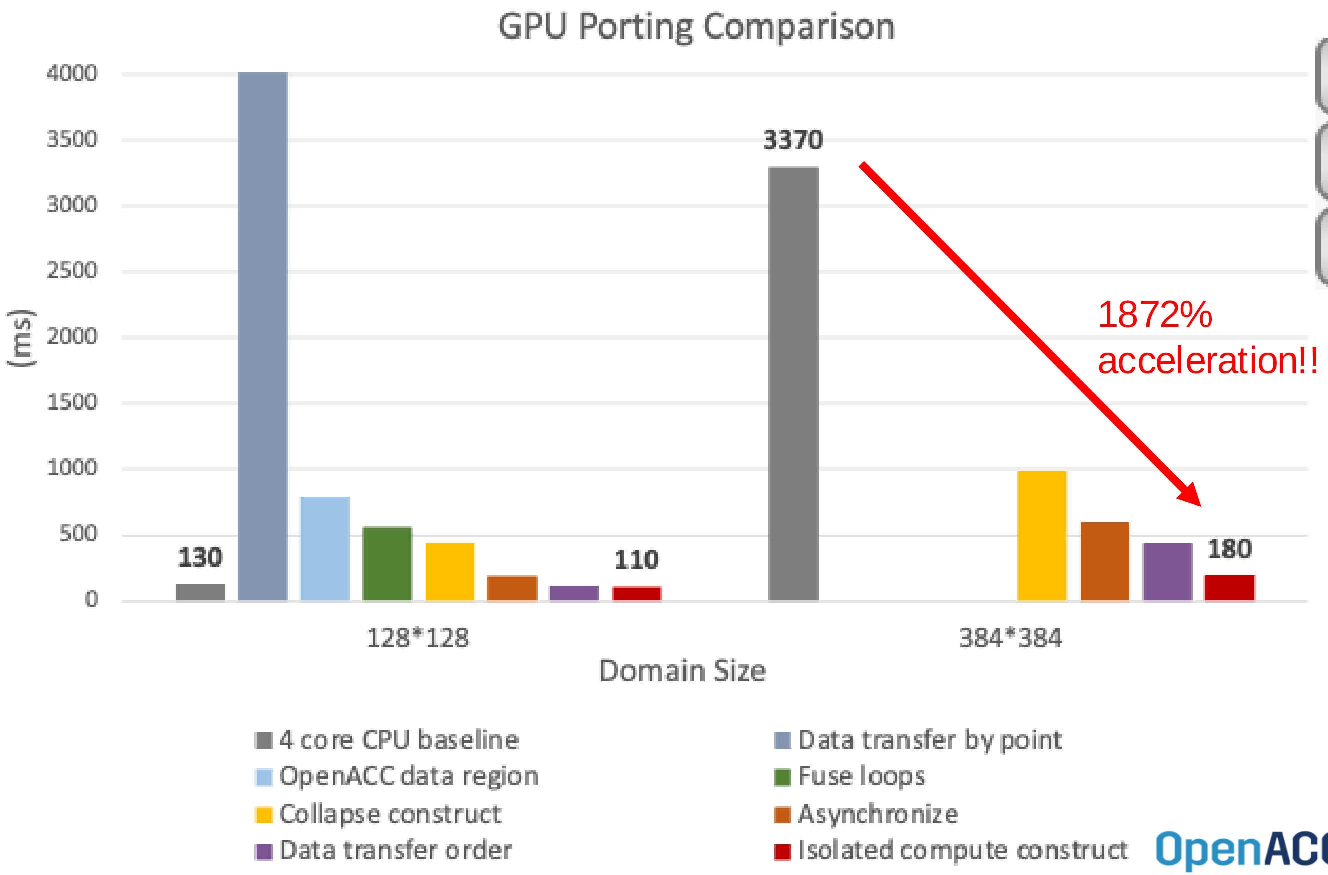


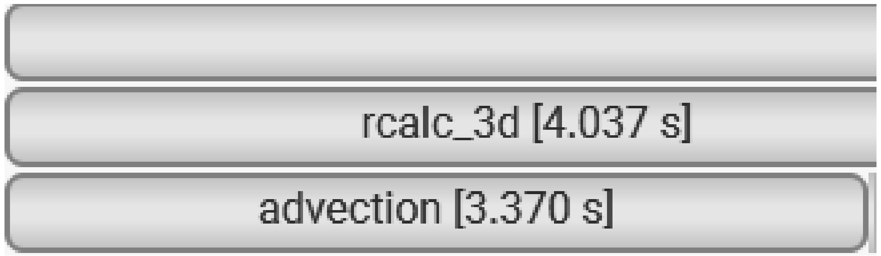
- **Improve data locality:**
- Pre-load reusable data before calling the advection module and present them in the module
- Create local variables in the GPU memory
- pruning legacy codes: reduce loops from 19 to 8
- asynchronize multiple loops

Results and Final Profile

GPU







4-core CPU

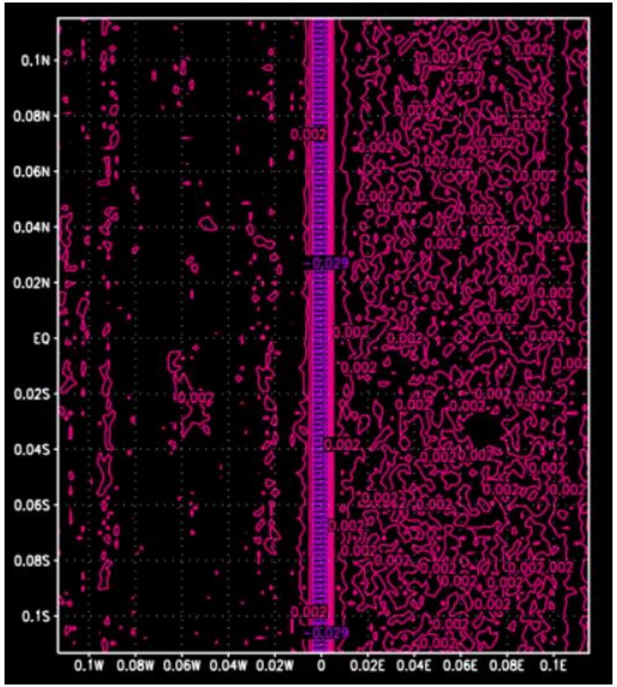
Energy Efficiency

INPUTS			
# CPU Cores	4		
# GPUs (A100)	1		
Application Speedup	18.7x		
Node Replacement	4.7x		
GPU NODE POWER SAVINGS			
	AMD Dual Rome 7742	8x A100 80GB SXM4	Power Savings
Compute Power (W)	5,143	6,500	-1,358
Networking Power (W)	217	93	124
Total Power (W)	**5,360**	**6,593**	-1,233
Node Power efficiency	**0.8x**		
ANNUAL ENERGY SAVINGS PER GPU NODE			
	AMD Dual Rome 7742	8x A100 80GB SXM4	Power Savings
Compute Power (kWh/year)	45,048	56,940	(11,892)
Networking Power (kWh/year)	1,902	814	1,088
Total Power (kWh/year)	**46,950**	**57,754**	**(10,804)**
$/kWh	0.20		
Annual Cost Savings	(2,160.71)		
3-year Cost Savings	(6,482.13)		
Metric Tons of CO_2	(8)		
Gasoline Cars Driven for 1 year	(2)		
Seedlings Trees grown for 10 years	(127)		

- **Time consumption of advection in one time step**
- **GPU acceleration is more apparent in larger-domain-computation**
- **We're able to achieve over 1860% speedup in the 384*384 domain.**
- **TaiwanVVM with 1024*1024 domain can achieve over 750% speedup in a sample test.**

unsolved problems: update_chemical module

- precision issues (not sure)




```fortran
subroutine ITER(gdt,k)
implicit none

  real    gdt
  integer k
  integer j,n,r,s  !loop count
  real :: YP_local(1:i1,1:j1), YL_local(1:i1,1:j1)

  YL_local = 0.
  YP_local = 0.
  !$acc data copyin(PL_scheme, KeffT, keff, RC, ysum, gdt, k, H2O) copy(ynew, YP, YL)
  !$acc parallel loop private(j, kreact,YP_local,YL_local)
  do n=1,nchsp  !chemical species
  if (PL_scheme(n)%active .EQV. .TRUE.) then    !reactive or not (True or False)
    if (PL_scheme(n)%name == H2O%name )  cycle    !don't do calculation of H2O
    do j=1, PL_scheme(n)%nr_PL     !chemical reactions (depend on chemical speices)
      if (RC(PL_scheme(n)%PL(j)%r_nr)%raddep == 1 ) then     !photolysis or not (1 or 0)
        select case (PL_scheme(n)%PL(j)%formula)      !select case of different formulas (8 types)
        case (0)
          if(PL_scheme(n)%PL(j)%PorL == 1) then    !production or loss (1 or 0)
              YP_local = YP_local + PL_scheme(n)%PL(j)%coef * keff(:,:,RC(PL_scheme(n)%PL(j)%r_nr)%Kindex,k)  !Production
          else
              YL_local = YL_local + PL_scheme(n)%PL(j)%coef * keff(:,:,RC(PL_scheme(n)%PL(j)%r_nr)%Kindex,k)  !Loss
          endif
        case (1~7) !other cases
        end select
      endif
    enddo   !end of chemical reactions
    do r=1,i1
      do s=1,j1
        !$acc atomic
        YP(r,s,n) = YP(r,s,n) + YP_local(r,s) !data output
        !$acc atomic
        YL(r,s,n) = YL(r,s,n) + YL_local(r,s) !data output
      enddo
    enddo
    ynew(:,:,n) = max(0.0,(ysum(:,:,n)+gdt*YP(:,:,n))/(1.0+gdt*YL(:,:,n))) !data output
  else
    ynew(:,:,n) = ysum(:,:,n)
  endif
  enddo   !end of chemical species
  !$acc end data
end subroutine ITER
```

ITT=12: `Contouring: -0 to 0.00012 interval 1e-05`

ITT=360: `Contouring: -0.016 to 0.001 interval 0.001`

ITT=720: `Contouring: -0.03 to 0.004 interval 0.001`

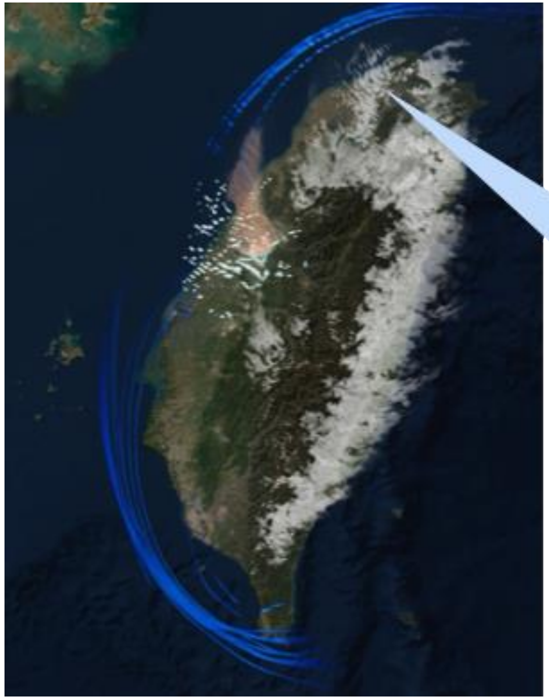
Wishlist and future plans

- keep working on update_chemical module
- focus on solving elliptical equations using CUDA
- cuSPARSE or cuFFT

$$\mu \frac{\partial w}{\partial t} + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) w + \frac{\partial}{\partial z}\left[\frac{1}{\rho_0}\frac{\partial}{\partial z}(\rho_0 w)\right] = -\frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \qquad \text{(A.6)}$$

(Wu and Arakawa, 2011)

以GPU加速計算建構臺灣天氣的數位孿生



GBA-VVM團隊來自臺灣大學雲動力模擬暨大氣環境實驗室，將 VVM加速了18倍！！

天氣與生活息息相關，從日常是否帶傘到空汙政策規劃都需仰賴氣象資訊。臺灣地狹人稠，對劇烈天氣的時機、強度與影響範圍的掌握尤為重要。VVM是一個優異的高解析度大氣模式，能有效模擬臺灣常見的午後雷陣雨及空污天氣，但其預報模擬需大量CPU運算，受限於硬體資源有限常導致模擬時間過長，難以提供即時預報參考，且高耗能的計算亦不符合減碳趨勢。為此，將VVM運算改由GPU加速，不僅縮短模擬時間，也符合減能需求。透過程式重整與清理降低計算複雜度，並以GPU進行VVM中氣象參數及污染物的傳送計算，實現了18倍的加速效果。此成果與開發經驗有助於提升VVM其他模組效能，並將VVM轉型為以GPU為核心的高速運算氣象模式，為建構臺灣天氣數位孿生系統奠定關鍵基礎。

Optimize data management

Optimize program construct

	4 core CPU baseline	Data transfer by point	OpenACC data region	Fuse loops	Collapse construct	Asynchronize directional advection	Change data transfer order	Isolated compute construct
128*128	130	7300(--)	790(--)	560(--)	440(--)	190(--)	120(1.08x)	110(1.18x)
384*384	3370				985(3.42x)	600(5.62x)	440(7.66x)	180(18.72x)

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Thank You

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