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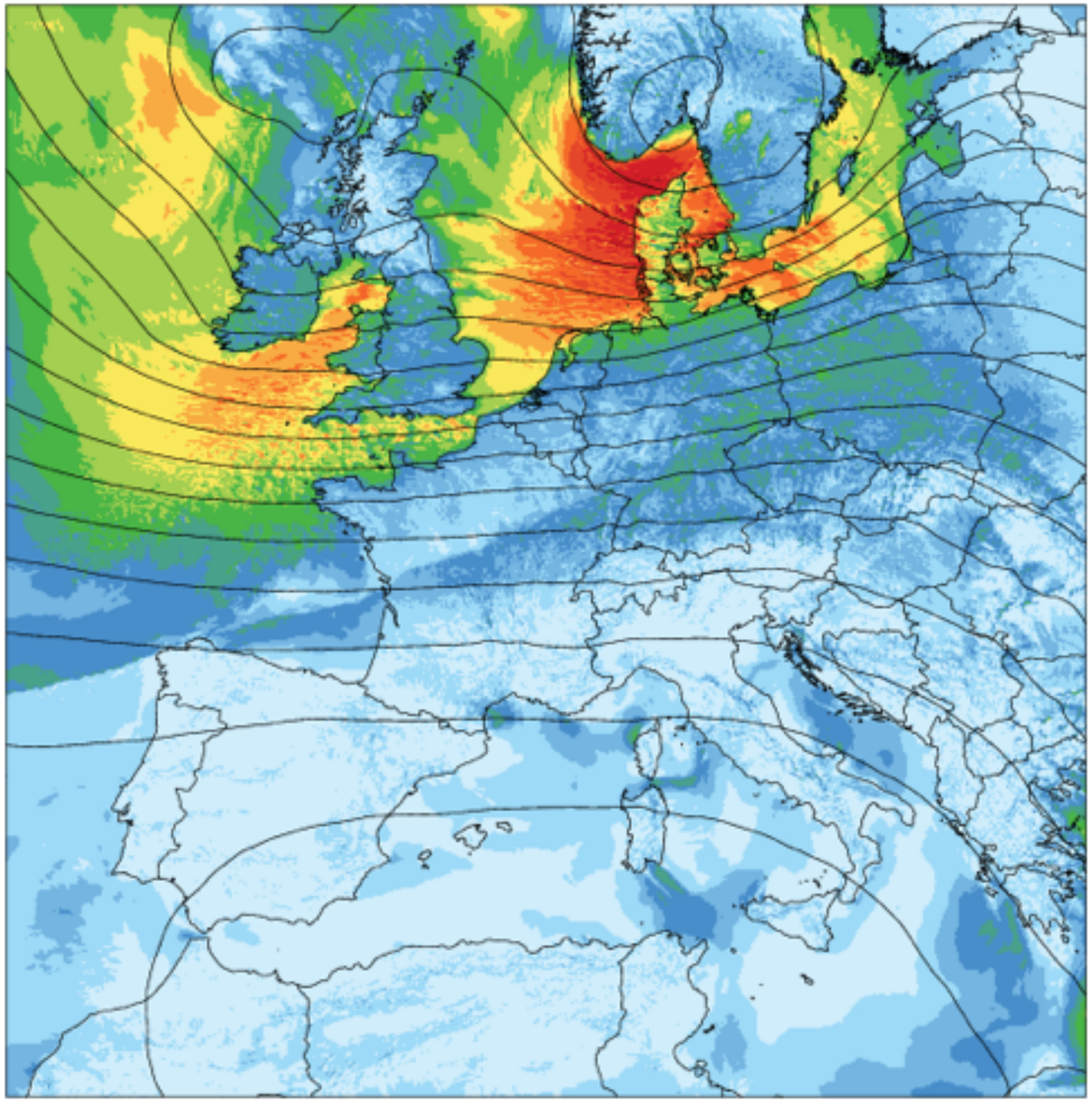
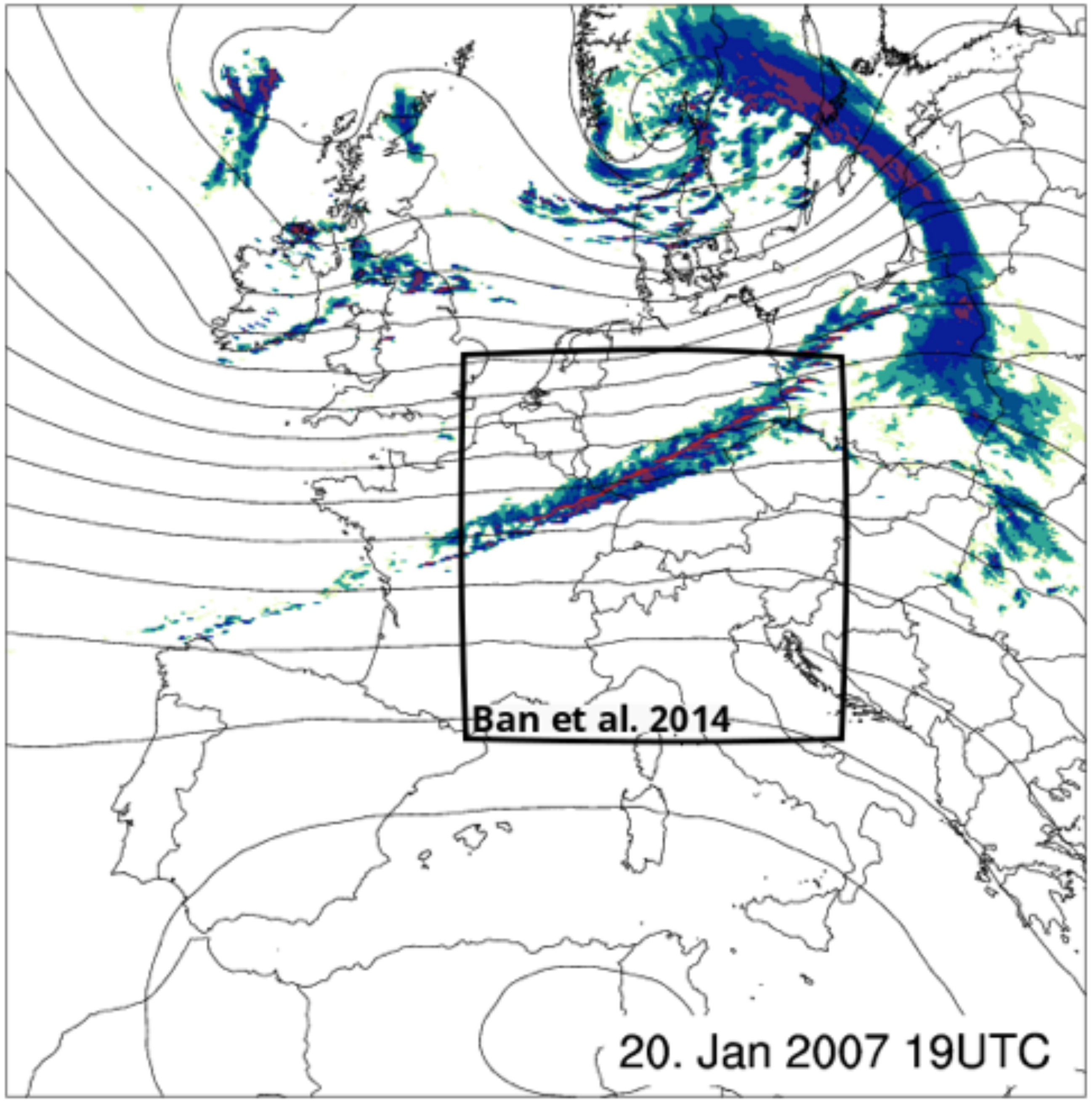
The challenges of new, efficient computer architectures, and how they can be met with a scalable software development strategy

Thomas C. Schulthess

"Piz Daint," presently one of Europe's most powerful petascale supercomputers

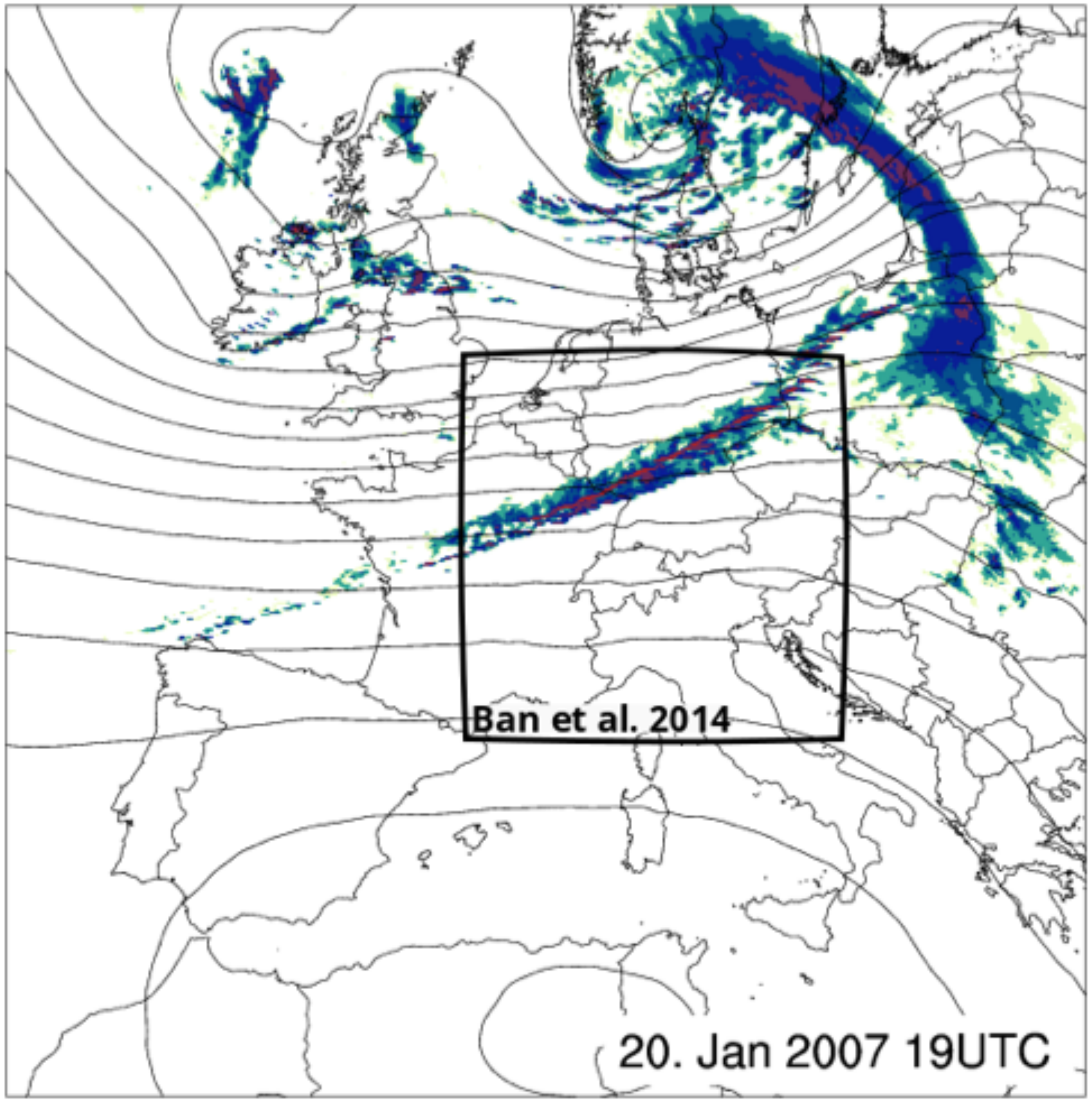
Cray XC30 with 5272 hybrid nodes:
Intel SandyBridge CPU + NVIDIA K20x GPU





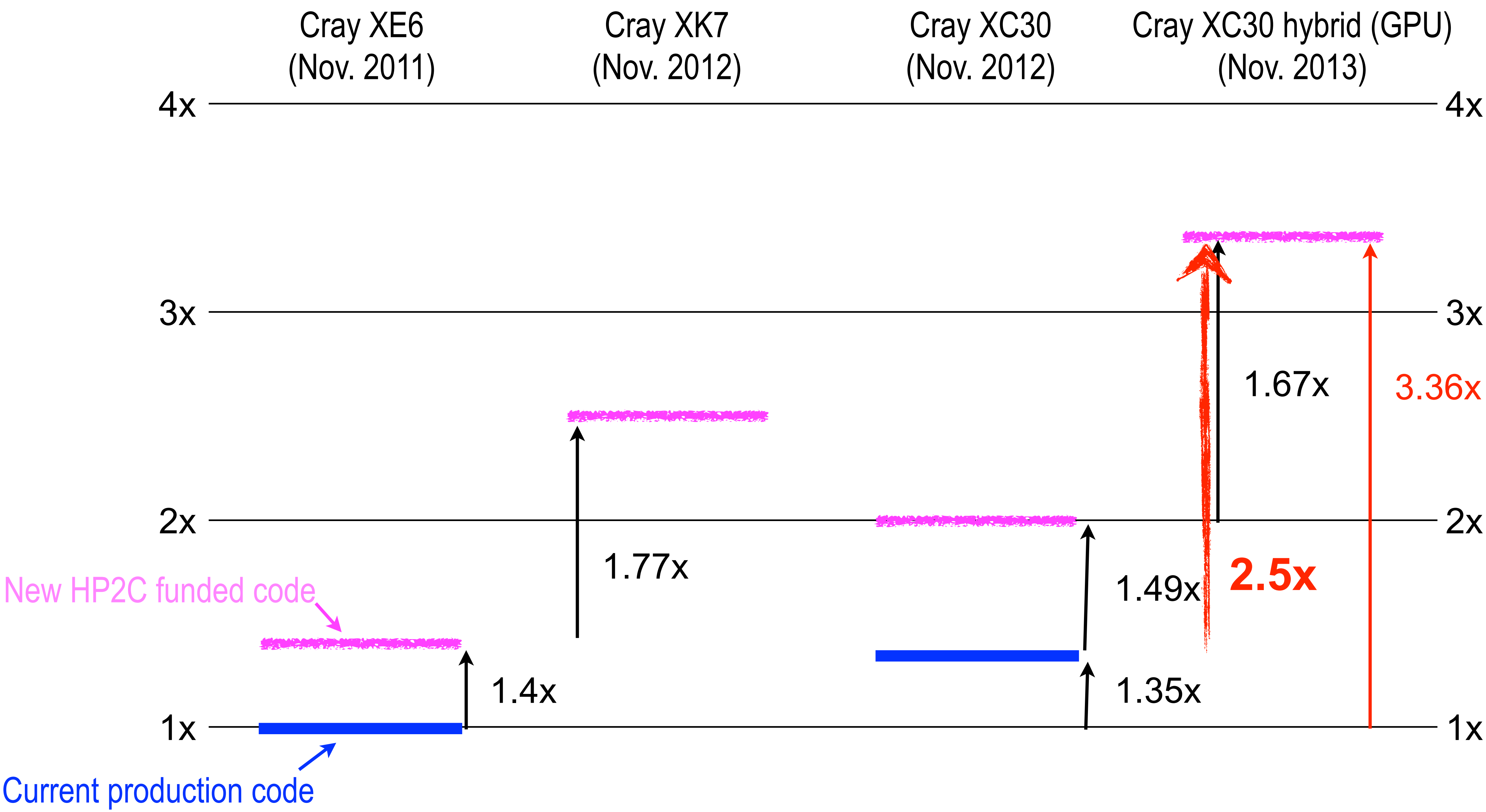
source: David Leutwyler

- Domain is larger by ~ 10x
  - small: 500 x 500 x 60
  - large: 1536 x 1536 x 60
- Same integration speed 1:80
- About 1.5x more nodes
  - small: 95 nodes @ 32 (AMD) cores
  - large: 144 hybrid (GPU+CPU) nodes
- Different implementations
  - small: regular COSMO code (MPI)
  - large: new MPI+OpenMP/CUDA code

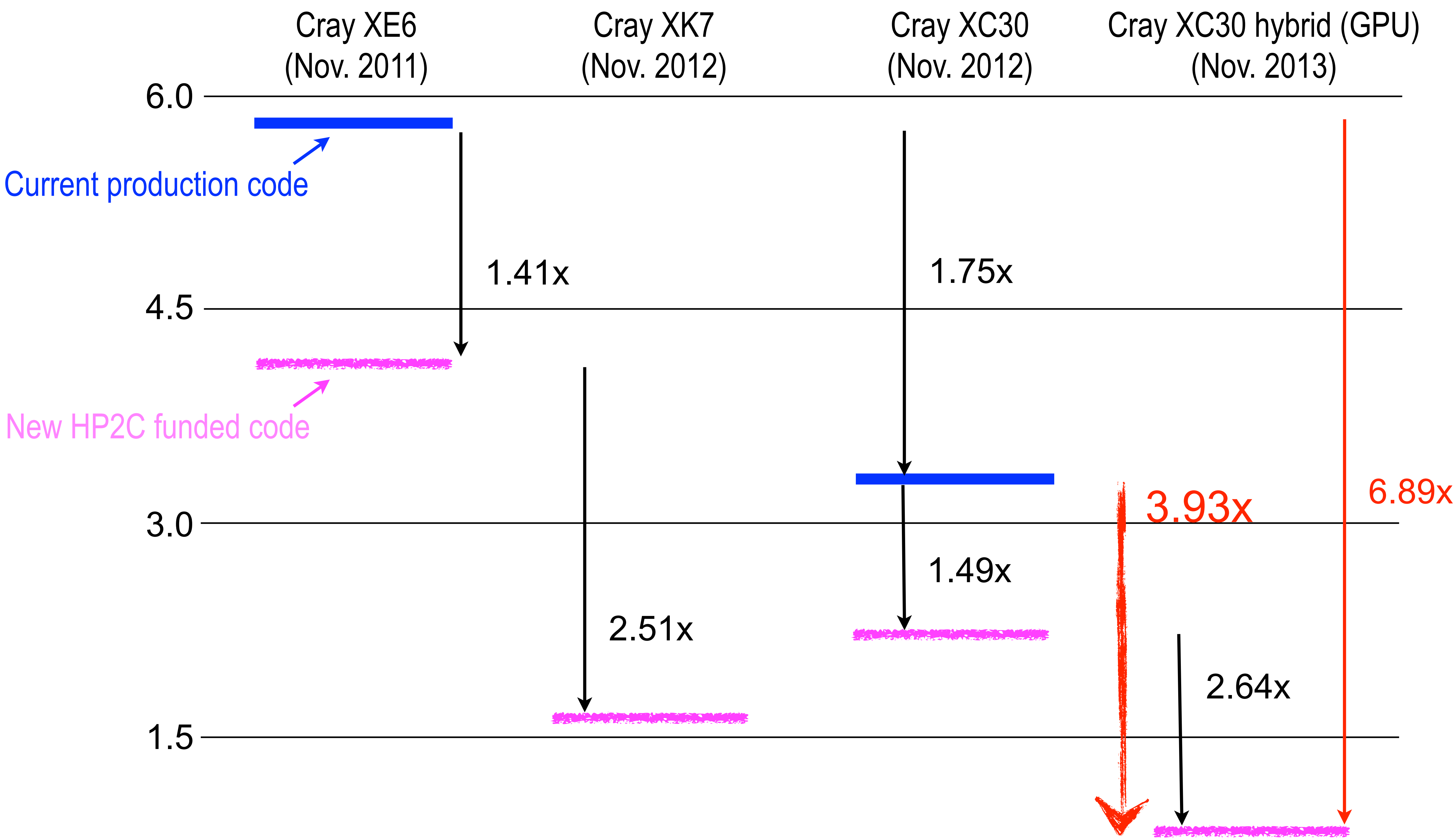


source: David Leutwyler

Speedup of the full COSMO-2 production problem (apples to apples with 33h forecast of Meteo Swiss)



Energy to solution (kWh / ensemble member)



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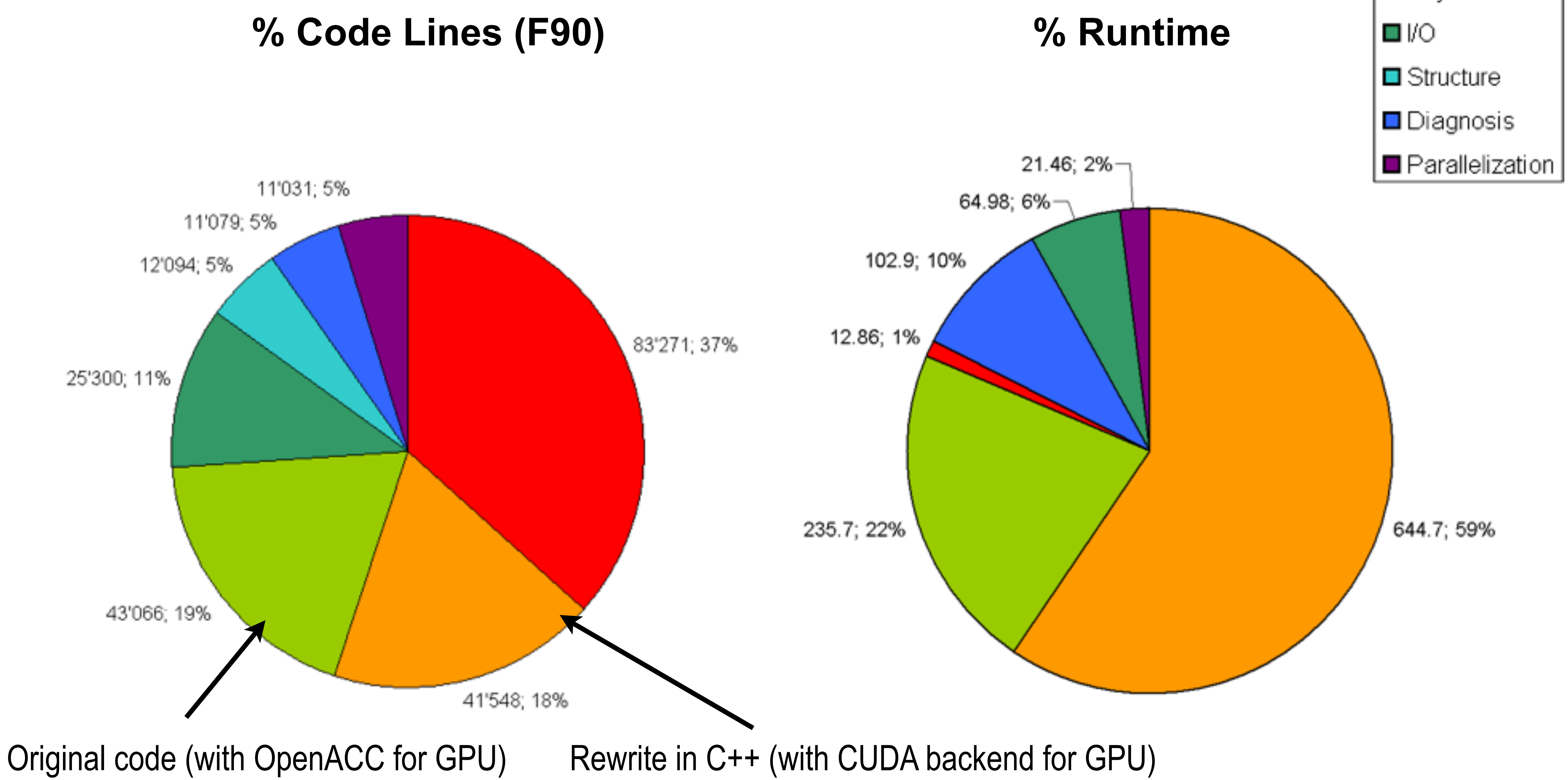
The bottom line: Improving the implementation and introducing a new architecture (GPUs) results in a 2 1/2 x speedup and 4 x improvement in energy to solution

Refactoring COSMO

Runtime based 2 km production model of MeteoSwiss



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velocities

$$\frac{\partial u}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\frac{\partial E_h}{\partial\lambda} - vV_a\right\} - \dot{\zeta}\frac{\partial u}{\partial\zeta} - \frac{1}{\rho a\cos\varphi}\left(\frac{\partial p'}{\partial\lambda} - \frac{1}{\sqrt{\gamma}}\frac{\partial p_0}{\partial\lambda}\frac{\partial p'}{\partial\zeta}\right) + M_u$$

$$\frac{\partial v}{\partial t} = -\left\{\frac{1}{a}\frac{\partial E_h}{\partial\varphi} + uV_a\right\} - \dot{\zeta}\frac{\partial v}{\partial\zeta} - \frac{1}{\rho a}\left(\frac{\partial p'}{\partial\varphi} - \frac{1}{\sqrt{\gamma}}\frac{\partial p_0}{\partial\varphi}\frac{\partial p'}{\partial\zeta}\right) + M_v$$

$$\frac{\partial w}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial w}{\partial\lambda} + v\cos\varphi\frac{\partial w}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial w}{\partial\zeta} + \frac{g}{\sqrt{\gamma}}\frac{\rho_0}{\rho}\frac{\partial p'}{\partial\zeta} + M_w + g\frac{\rho_0}{\rho}\left\{\frac{(T-T_0)}{T} - \frac{T_0 p'}{T p_0} + \left(\frac{R_v}{R_d} - 1\right)q^v - q^l - q^f\right\}$$

pressure

$$\frac{\partial p'}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial p'}{\partial\lambda} + v\cos\varphi\frac{\partial p'}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial p'}{\partial\zeta} + g\rho_0 w - \frac{c_{pd}}{c_{vd}}pD$$

temperature

$$\frac{\partial T}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial T}{\partial\lambda} + v\cos\varphi\frac{\partial T}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial T}{\partial\zeta} - \frac{1}{\rho c_{vd}}pD + Q_T$$

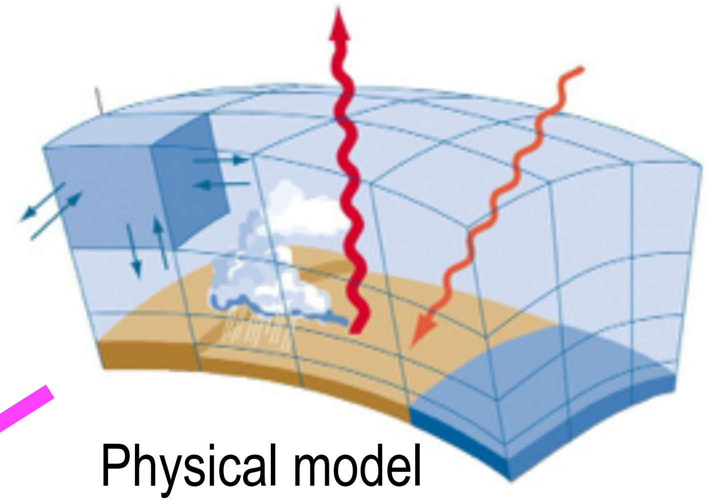
water

$$\frac{\partial q^v}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial q^v}{\partial\lambda} + v\cos\varphi\frac{\partial q^v}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial q^v}{\partial\zeta} - (S^l + S^f) + M_{q^v}$$

$$\frac{\partial q^{l,f}}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial q^{l,f}}{\partial\lambda} + v\cos\varphi\frac{\partial q^{l,f}}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial q^{l,f}}{\partial\zeta} - \frac{g}{\sqrt{\gamma}}\frac{\rho_0}{\rho}\frac{\partial P_{l,f}}{\partial\zeta} + S^{l,f} + M_{q^{l,f}}$$

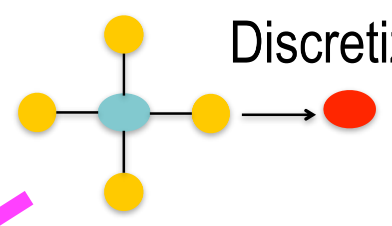
turbulence

$$\frac{\partial e_t}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial e_t}{\partial\lambda} + v\cos\varphi\frac{\partial e_t}{\partial\varphi}\right)\right\} - \dot{\zeta}\frac{\partial e_t}{\partial\zeta} + K_m^v\frac{g\rho_0}{\sqrt{\gamma}}\left\{\left(\frac{\partial u}{\partial\zeta}\right)^2 + \left(\frac{\partial v}{\partial\zeta}\right)^2\right\} + \frac{g}{\rho\theta_v}F^{\theta_v} - \frac{\sqrt{2}e_t^{3/2}}{\alpha_M l} + M_{e_t}$$



Physical model

Mathematical description



Discretization / algorithm

Domain science (incl. applied mathematics)

```
lap(i,j,k) = -4.0 * data(i,j,k) +
    data(i+1,j,k) + data(i-1,j,k) +
    data(i,j+1,k) + data(i,j-1,k);
```

Code / implementation

Code compilation

A given supercomputer

“Port” serial code to supercomputers
- > vectorize
- > parallelize
- > petascaling
- > exascaling
- > ...

Computer engineering (& computer science)

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

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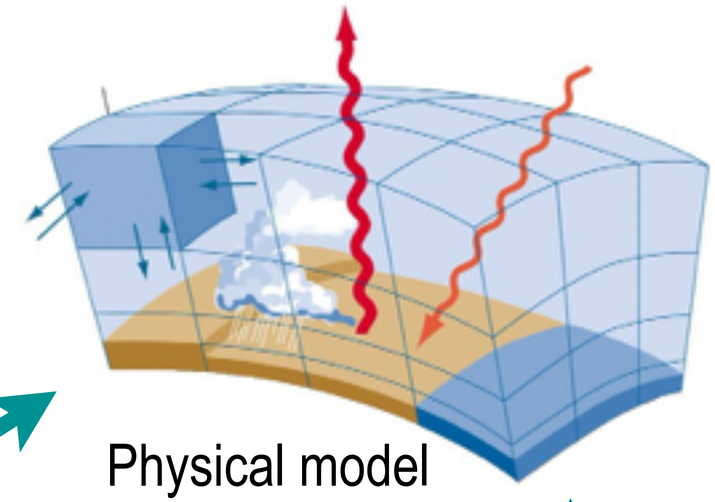
$$\text{velocities}\begin{cases}\dfrac{\partial u}{\partial t} = -\left\{\dfrac{1}{a\cos\varphi}\dfrac{\partial E_h}{\partial\lambda} - vV_a\right\} - \dot\zeta\dfrac{\partial u}{\partial\zeta} - \dfrac{1}{\rho a\cos\varphi}\left(\dfrac{\partial p'}{\partial\lambda} - \dfrac{1}{\sqrt{\gamma}}\dfrac{\partial p_0}{\partial\lambda}\dfrac{\partial p'}{\partial\zeta}\right) + M_u \\ \dfrac{\partial v}{\partial t} = -\left\{\dfrac{1}{a}\dfrac{\partial E_h}{\partial\varphi} + uV_a\right\} - \dot\zeta\dfrac{\partial v}{\partial\zeta} - \dfrac{1}{\rho a}\left(\dfrac{\partial p'}{\partial\varphi} - \dfrac{1}{\sqrt{\gamma}}\dfrac{\partial p_0}{\partial\varphi}\dfrac{\partial p'}{\partial\zeta}\right) + M_v \\ \dfrac{\partial w}{\partial t} = -\left\{\dfrac{1}{a\cos\varphi}\left(u\dfrac{\partial w}{\partial\lambda} + v\cos\varphi\dfrac{\partial w}{\partial\varphi}\right)\right\} - \dot\zeta\dfrac{\partial w}{\partial\zeta} + \dfrac{g}{\sqrt{\gamma}}\dfrac{\rho_0}{\rho}\dfrac{\partial p'}{\partial\zeta} + M_w + g\dfrac{\rho_0}{\rho}\left\{\dfrac{(T-T_0)}{T} - \dfrac{T_0 p'}{T p_0} + \left(\dfrac{R_v}{R_d} - 1\right)q^v - q^l - q^f\right\}\end{cases}$$

$$\text{pressure}\quad \frac{\partial p'}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial p'}{\partial\lambda} + v\cos\varphi\frac{\partial p'}{\partial\varphi}\right)\right\} - \dot\zeta\frac{\partial p'}{\partial\zeta} + g\rho_0 w - \frac{c_{pd}}{c_{vd}}pD$$

$$\text{temperature}\quad \frac{\partial T}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial T}{\partial\lambda} + v\cos\varphi\frac{\partial T}{\partial\varphi}\right)\right\} - \dot\zeta\frac{\partial T}{\partial\zeta} - \frac{1}{\rho c_{vd}}pD + Q_T$$

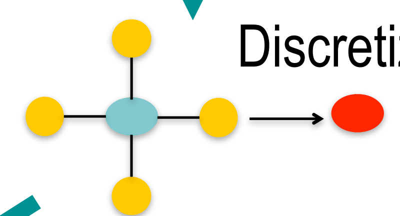
$$\text{water}\begin{cases}\dfrac{\partial q^v}{\partial t} = -\left\{\dfrac{1}{a\cos\varphi}\left(u\dfrac{\partial q^v}{\partial\lambda} + v\cos\varphi\dfrac{\partial q^v}{\partial\varphi}\right)\right\} - \dot\zeta\dfrac{\partial q^v}{\partial\zeta} - (S^l + S^f) + M_{q^v} \\ \dfrac{\partial q^{l,f}}{\partial t} = -\left\{\dfrac{1}{a\cos\varphi}\left(u\dfrac{\partial q^{l,f}}{\partial\lambda} + v\cos\varphi\dfrac{\partial q^{l,f}}{\partial\varphi}\right)\right\} - \dot\zeta\dfrac{\partial q^{l,f}}{\partial\zeta} - \dfrac{g}{\sqrt{\gamma}}\dfrac{\rho_0}{\rho}\dfrac{\partial P_{l,f}}{\partial\zeta} + S^{l,f} + M_{q^{l,f}}\end{cases}$$

$$\text{turbulence}\quad \frac{\partial e_t}{\partial t} = -\left\{\frac{1}{a\cos\varphi}\left(u\frac{\partial e_t}{\partial\lambda} + v\cos\varphi\frac{\partial e_t}{\partial\varphi}\right)\right\} - \dot\zeta\frac{\partial e_t}{\partial\zeta} + K_m^v\frac{g\rho_0}{\sqrt{\gamma}}\left\{\left(\frac{\partial u}{\partial\zeta}\right)^2 + \left(\frac{\partial v}{\partial\zeta}\right)^2\right\} + \frac{g}{\rho\theta_v}F^{\theta_v} - \frac{\sqrt{2}e_t^{3/2}}{\alpha_M l} + M_{e_t}$$



Physical model

Mathematical description



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```

Code / implementation

Domain specific libraries & tools

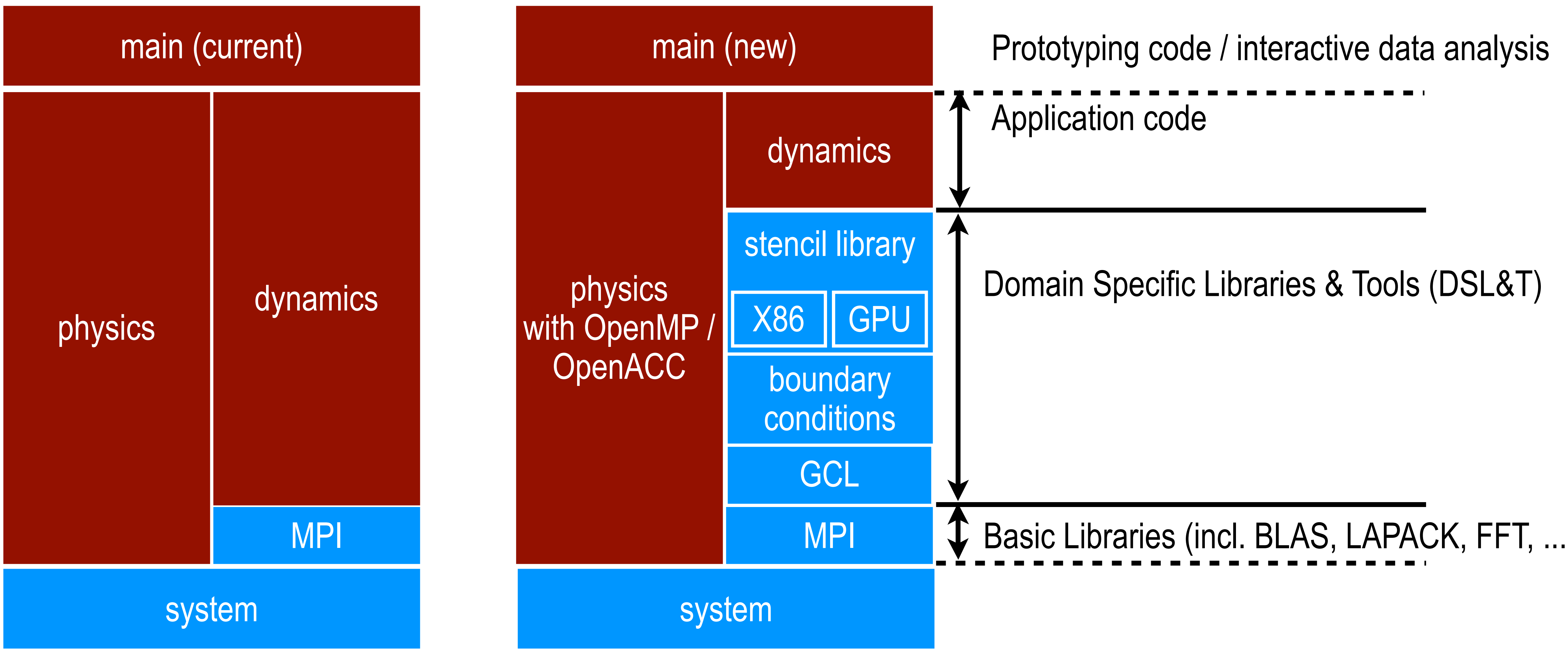
Code compilation

Optimal algorithm
Auto tuning

Architectural options / design

Computer engineering (& computer science)

COSMO: current and new, HP2C developed code



Gory detail will be given in Xavier's talk tomorrow

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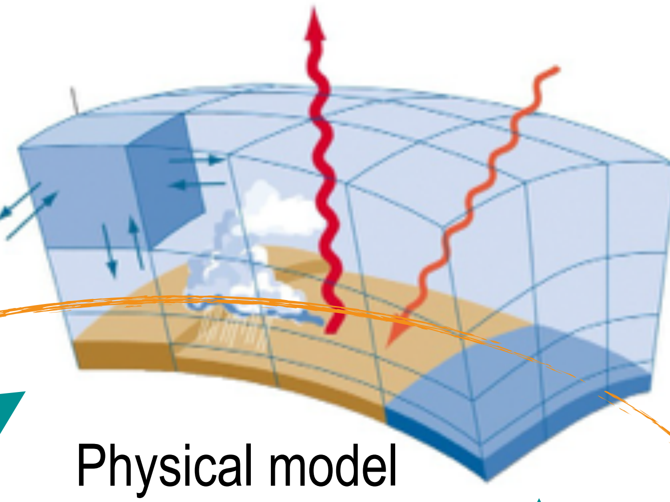
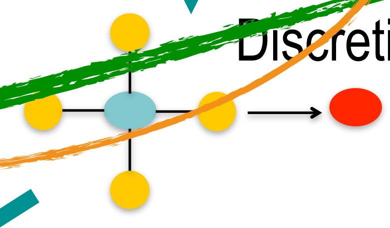


Physical model

Mathematical description

Dynamic developer environment, i.e. not Fortran/C/C++ but based on Python or equivalent dynamic language



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```

Code / implementation

Domain specific libraries & tools

Code compilation

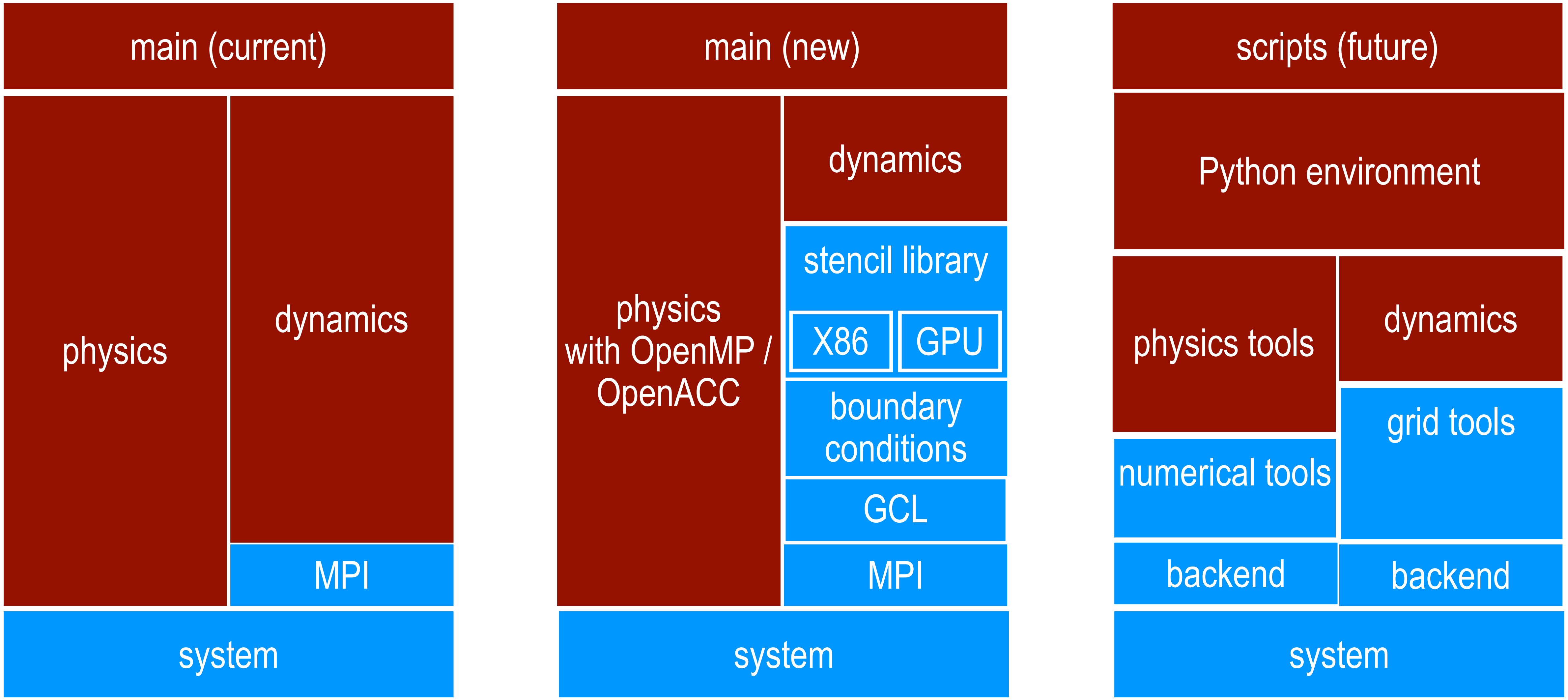
Optimal algorithm
Auto tuning

PASC co-design projects

Computer engineering (& computer science)

Architectural options / design

COSMO & other models: how things could develop with a dynamic developer environment



The main advantage: model development is scalable!

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THANK YOU!